Effect of a Locally Repulsive Interaction on s–wave Superconductors

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Abstract

The thermodynamic impact of the Coulomb repulsion on s–wave superconductors is analyzed via a rigorous study of equilibrium and ground states of the strong coupling BCS–Hubbard Hamiltonian. We show that the one–site electron repulsion can favor superconductivity at fixed chemical potential by increasing the critical temperature and/or the Cooper pair condensate density. If the one–site repulsion is not too large, a first or a second order superconducting phase transition can appear at low temperatures. The Meißner effect is shown to be rather generic but coexistence of superconducting and ferromagnetic phases is also shown to be feasible, for instance near half–filling and at strong repulsion. Our proof of a superconductor–Mott insulator phase transition implies a rigorous explanation of the necessity of doping insulators to create superconductors. These mathematical results are consequences of "quantum large deviation" arguments combined with an adaptation of the proof of Størmer's theorem [1] to even states on the CAR algebra.

Keywords: Superconductivity – s–wave – Coulomb interaction – Hubbard model – Meißner effect – Mott insulators – Equilibrium states – Størmer's theorem

1. Introduction

Since the discovery of mercury superconductivity in 1911 by the Dutch physicist Onnes, the study of superconductors has continued to intensify, see, e.g., [2]. Since that discovery, a significant amount of superconducting materials has been found. This includes usual metals, like lead, aluminum, zinc or platinum, magnetic materials, heavy–fermion systems, organic compounds and ceramics. A complete description of their thermodynamic properties is an entire subject by itself, see [2, 3, 4] and references therein. In addition to zero–resistivity and many other complex phenomena, superconductors manifest the celebrated Meißner or Meißner–Ochsenfeld effect, i.e., they can become perfectly diamagnetic. The highest[1] critical temperature for superconductivity obtained nowadays is between 100 and 200 Kelvin via doped copper oxides, which are originally insulators. In contrast to most superconductors, note that superconduction in magnetic superconductors only exists on a finite range of non–zero temperatures.

Theoretical foundations of superconductivity go back to the celebrated BCS theory – appeared in the late fifties (1957) – which explains conventional type I superconductors. This theory is based on the so–called (reduced) BCS Hamiltonian

$$\mathrm{H}_{\Lambda}^{BCS} := \sum_{k\in\Lambda^*} (\varepsilon_k - \mu)\left(\tilde{a}_{k,\uparrow}^*\tilde{a}_{k,\uparrow} + \tilde{a}_{k,\downarrow}^*\tilde{a}_{k,\downarrow}\right) + \frac{1}{|\Lambda|}\sum_{k,k'\in\Lambda^*}\gamma_{k,k'}\tilde{a}_{k,\uparrow}^*\tilde{a}_{-k,\downarrow}^*\tilde{a}_{k',\downarrow}\tilde{a}_{-k',\uparrow} \tag{1.1}$$

defined in a cubic box $\Lambda \subset \mathbb{R}^3$ of volume $|\Lambda|$. Here Λ^* is the dual group of Λ seen as a torus (periodic boundary condition) and the operator $\tilde{a}_{k,s}^*$ resp. $\tilde{a}_{k,s}$ creates resp. annihilates a fermion with spin $s \in \{\uparrow,\downarrow\}$ and momentum $k \in \Lambda^*$. The function ε_k represents the kinetic energy, the real number μ is the chemical

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[1] In January 2008, a critical temperature over 180 Kelvin was reported in a Pb-doped copper oxide.

potential and $\gamma_{k,k'}$ is the BCS coupling function. The choice $\gamma_{k,k'} = -\gamma < 0$ is often used in the Physics literature and the case $\varepsilon_k = 0$ is known as the strong coupling limit of the BCS model.

The lattice approximation of the BCS Hamiltonian amounts to replace the box $\Lambda \subset \mathbb{R}^3$ by $\Lambda \subset \mathbb{Z}^3$ (or more generally by $\Lambda \subset \mathbb{Z}^{d\geq 1}$) and the strong coupling limit of the reduced BCS model is in this case known as the strong coupling (with $\gamma_{k,k'} = -\gamma$) BCS model[2]. The assumptions $\epsilon_k = 0$ and $\gamma_{k,k'} = -\gamma$ are of interest, because in this case the BCS Hamiltonian can be explicitly diagonalised. The exact solution of the strong coupling BCS model is well–known since the sixties [6, 7]. This model is in a sense unrealistic: among other things, its representation of the kinetic energy of electrons is rather poor. Nevertheless it became popular because it displays most of basic properties of real conventional type I superconductors. See, e.g., Chapter VII, Section 4 in [8]. Even though the analysis of the thermodynamics of the BCS Hamiltonian was rigorously performed in the eighties [9, 10] (see also the innovating work of Bernadskii and Minlos in 1972 [11]), generalizations of the strong coupling approximation of the BCS model are still subject of research. For instance, strong coupling–BCS–type models with superconducting phases at arbitrarily high temperatures are treated in [12].

In fact, a general theory of superconductivity is still a subject of debate, especially for high–T_c superconductors. An important phenomenon ignored in the BCS theory is the Coulomb interaction between electrons or holes, which can imply strong correlations, for instance in high–T_c superconductors. To study these correlations, most of theoretical methods, inspired by Beliaev [5], use perturbation theory or renormalization group derived from the diagram approach of Quantum Field Theory. However, even if these approaches have been successful in explaining many physical properties of superconductors [3, 4], only few rigorous results exist on superconductivity.

For instance, the effect of the Coulomb interaction on superconductivity is not rigorously known. This problem was of course adressed in theoretical Physics right after the emergence of the Fröhlich model and the BCS theory, see, e.g., [13]. In particular, the authors explain in [13, Chapter VI], by means of diagrammatic pertubation theory, that the effect of the Coulomb interaction on the Fröhlich model should be to lower the critical temperature of the superconducting phase by lowering the electron density. We rigorously show that this phenomenology is only true – for our model – in a specific region of parameters.

Indeed, the aim of the present paper is to understand the possible thermodynamic impact of the Coulomb repulsion in the strong coupling approximation. More precisely, we study the thermodynamic properties of the strong coupling BCS–Hubbard model defined in the box[3] $\Lambda_N := \{\mathbb{Z} \cap [-L, L]\}^{d\geq 1}$ of volume $|\Lambda_N| = N \geq 2$ by the Hamiltonian

$$\begin{aligned} \mathrm{H}_N := \quad & -\mu \sum_{x\in\Lambda_N} (n_{x,\uparrow} + n_{x,\downarrow}) - h \sum_{x\in\Lambda_N} (n_{x,\uparrow} - n_{x,\downarrow}) + 2\lambda \sum_{x\in\Lambda_N} n_{x,\uparrow} n_{x,\downarrow} \\ & - \frac{\gamma}{N} \sum_{x,y\in\Lambda_N} a^*_{x,\uparrow} a^*_{x,\downarrow} a_{y,\downarrow} a_{y,\uparrow} \end{aligned} \tag{1.2}$$

for real parameters μ, h, λ, and $\gamma \geq 0$. The operator $a^*_{x,s}$ resp. $a_{x,s}$ creates resp. annihilates a fermion with spin $s \in \{\uparrow, \downarrow\}$ at lattice position $x \in \mathbb{Z}^d$ whereas $n_{x,s} := a^*_{x,s} a_{x,s}$ is the particle number operator at position x and spin s. The first term of the right hand side (r.h.s.) of (1.2) represents the strong coupling limit of the kinetic energy, with μ being the chemical potential of the system. Note that this "strong coupling limit" – explained above for the BCS Hamiltonian – is also called "atomic limit" in the context of the Hubbard model, see, e.g., [14, 15]. The second term in the r.h.s. of (1.2) corresponds to the interaction between spins and the magnetic field h. The one–site interaction with coupling constant λ represents the (screened) Coulomb repulsion as in the celebrated Hubbard model. So, the parameter λ should be taken as a positive number but our results are also valid for any real λ. The last term is the BCS interaction written in the x–space since

$$\frac{\gamma}{N} \sum_{x,y\in\Lambda_N} a^*_{x,\uparrow} a^*_{x,\downarrow} a_{y,\downarrow} a_{y,\uparrow} = \frac{\gamma}{N} \sum_{k,q\in\Lambda^*_N} \tilde{a}^*_{k,\uparrow} \tilde{a}^*_{-k,\downarrow} \tilde{a}_{q,\downarrow} \tilde{a}_{-q,\uparrow}, \tag{1.3}$$

with Λ^*_N being the reciprocal lattice of quasi–momenta and where $\tilde{a}_{q,s}$ is the corresponding annihilation operator for $s \in \{\uparrow, \downarrow\}$. Observe that the thermodynamics of the model for $\gamma = 0$ can easily be computed. Therefore

[2] See also (1.2) with $\lambda = 0$ and $h = 0$.

[3] Without loss of generality we choose N such that $L := (N^{1/d} - 1)/2 \in \mathbb{N}$.

we restrict the analysis to the case $\gamma > 0$. Note also that the homogeneous BCS interaction (1.3) can imply a superconducting phase and the mediator implying this effective interaction does not matter here, i.e., it could be due to phonons, as in conventional type I superconductors, or anything else.

We show that the one–site repulsion suppresses superconductivity for large $\lambda \geq 0$. In particular, the repulsive term in (1.2) cannot imply any superconducting state if $\gamma = 0$. However, the first elementary but nonetheless important property of this model is that the presence of an electron repulsion is not incompatible with superconductivity if $|\lambda - \mu|$ and $(\lambda + |h|)$ are not too big as compared to the coupling constant γ of the BCS interaction. In this case, the superconducting phase appears at low temperatures as either a first order or a second order phase transition. More surprisingly, the one–site repulsion can even favor superconductivity at fixed chemical potential μ by increasing the critical temperature and/or the Cooper pair condensate density. This contradicts the naive guess that any one–site repulsion between electron pairs should at least reduce the formation of Cooper pairs. It is however important to mention that the physical behavior described by the model depends on which parameter, μ or ρ, is fixed. (It does not mean that the canonical and grand–canonical ensembles are not equivalent for this model). Indeed, we also analyze the thermodynamic properties at fixed electron density ρ per site in the grand–canonical ensemble, as it is done for the perfect Bose gas in the proof of Bose-Einstein condensation. The analysis of the thermodynamics of the strong coupling BCS–Hubbard model is performed in details. In particular, we prove that the Meißner effect is rather generic but also that the coexistence of superconducting and ferromagnetic phases is possible (as in the Vonsovkii–Zener model [16, 17]), for instance at large $\lambda > 0$ and densities near half–filling. The later situation is related to a superconductor–Mott insulator phase transition. This transition gives furthermore a rigorous explanation of the need of doping insulators to obtain superconductors. Indeed, at large enough coupling constant λ, the superconductor–Mott insulator phase transition corresponds to the breakdown of superconductivity together with the appearance of a gap in the chemical potential as soon as the electron density per site becomes an integer, i.e., 0, 1 or 2. If the system has an electron density per site equal to 1 without being superconductor, then any non–zero magnetic field $h \neq 0$ implies a ferromagnetic phase.

Note that the present setting is still too simplified with respect to (w.r.t.) real superconductors. For instance, the anti–ferromagnetic phase or the presence of vortices, which can appear in (type II) high–T_c superconductors [3, 4], are not modeled. However, the BCS–Hubbard Hamiltonian (1.2) may be a good model for certain kinds of superconductors or ultra-cold Fermi gases in optical lattices, where the strong coupling approximation is experimentally justified. Actually, even if the strong coupling assumption is a severe simplification, it may be used in order to analyze the thermodynamic impact of the Coulomb repulsion, as all parameters of the model have a phenomenological interpretation and can be directly related to experiments. See discussions in Section 5. Moreover, the range of parameters in which we are interested turns out to be related to a first order phase transition. This kind of phase transitions are known to be stable under small perturbations of the Hamiltonian. In particular, by including a small kinetic part it can be shown by high–low temperature expansions that the model

$$\mathrm{H}_{N,\varepsilon} := \mathrm{H}_N + \sum_{x,y\in\Lambda_N} \varepsilon(x-y)\left(a_{y,\downarrow}^* a_{x,\downarrow} + a_{y,\uparrow}^* a_{x,\uparrow}\right)$$

has essentially the same correlation functions as H_N, up to corrections of order $||\varepsilon||_1$ (ℓ^1–norm of ε). This analysis will be the subject of a separated paper. For any $\varepsilon \neq 0$ notice that the model $\mathrm{H}_{N,\varepsilon}$ is not anymore permutation invariant but only translation invariant. Such translation invariant models are studied in a systematic way in [18]. Their detailed analysis is however, generally much more difficult to perform. Considering first models having more symmetries – as for instance, permutation invariance – is in this case technically easier.

Coming back to the strong coupling BCS–Hubbard model H_N, it turns out that the thermodynamic limit of its (grand–canonical) pressure[4]

$$\mathrm{p}_N(\beta,\mu,\lambda,\gamma,h) := \frac{1}{\beta N} \ln \mathrm{Trace}\left(e^{-\beta \mathrm{H}_N}\right) \tag{1.4}$$

exists at any fixed inverse temperature $\beta > 0$. It corresponds to a variational problem which has minimizers[5]

[4]Our notation for the "Trace" does not include the Hilbert space where it is evaluated but it should be deduced from operators involved in each statement.

[5]Because $\omega \mapsto \mathfrak{F}(\omega)$ is lower semicontinuous and $E_{\mathcal{U}}^{S,+}$ is compact with respect to the weak*–topology.

in the set $E_{\mathcal{U}}^{S,+}$ of (even[6]) permutation invariant states on the CAR C^*–algebra $\mathcal{U}$ generated by annihilation and creation operators:

$$\mathrm{p}\left(\beta,\mu,\lambda,\gamma,h\right):=\lim_{N\to\infty}\left\{\mathrm{p}_N\left(\beta,\mu,\lambda,\gamma,h\right)\right\}=-\inf_{\omega\in E_{\mathcal{U}}^{S,+}}\mathfrak{F}\left(\omega\right). \tag{1.5}$$

Here the map

$$\omega\mapsto\mathfrak{F}(\omega):=\mathfrak{e}(\omega)-\beta^{-1}\tilde{S}(\omega)$$

is the affine (lower weak*–semicontinuous) free–energy density functional defined on $E_{\mathcal{U}}^{S,+}$ from the mean energy per volume

$$\mathfrak{e}\left(\omega\right):=\lim_{N\to\infty}\left\{N^{-1}\omega\left(\mathrm{H}_N\right)\right\}<\infty$$

and the entropy density

$$\tilde{S}\left(\omega\right):=-\lim_{N\to\infty}\left\{\frac{1}{N}\mathrm{Trace}\left(D_{\omega|\mathcal{U}_N}\log D_{\omega|\mathcal{U}_N}\right)\right\}<\infty.$$

Note that $D_{\omega|\mathcal{U}_N}$ is the density matrix associated to the state ω restricted on the local CAR C^*–algebra $\mathcal{U}_N\simeq B\left(\bigwedge\mathbb{C}^{\Lambda_N\times\{\uparrow,\downarrow\}}\right)$ (isomorphism). Such a derivation of the pressure as a minimization problem over states on a C^*–algebras are also performed for various quantum spin systems, see, e.g., [19, 20, 21, 22, 23].

The minimum of the variational problem (1.5) is attained for any weak*–limit point of local Gibbs states

$$\omega_N\left(\cdot\right):=\frac{\mathrm{Trace}\left(\ \cdot\ e^{-\beta\mathrm{H}_N}\right)}{\mathrm{Trace}\left(e^{-\beta\mathrm{H}_N}\right)} \tag{1.6}$$

associated with H_N. Similarly to what is done for general translation invariant models (see [24, 25]), the set of *equilibrium states* of the strong coupling BCS–Hubbard model is naturally defined to be the set $\Omega_\beta=\Omega_\beta(\mu,\lambda,\gamma,h)$ of minimizers of (1.5). Note that Ω_β is a non empty convex subset[7] of $E_{\mathcal{U}}^{S,+}$ and the extremal decomposition in Ω_β coincides with the one in $E_{\mathcal{U}}^{S,+}$, i.e., Ω_β is a face[8] in $E_{\mathcal{U}}^{S,+}$. So, *pure* equilibrium states are extremal states of Ω_β. Meanwhile, any weak* limit point as $n\to\infty$ of an equilibrium state sequence $\{\omega^{(n)}\}_{n\in\mathbb{N}}$ with diverging inverse temperature $\beta_n\to\infty$ is – per definition – a *ground state* $\omega\in E_{\mathcal{U}}^{S,+}$.

Here we have left the Fock space representation of the model to go to a representation–free formulation of thermodynamic phases. This means that H_N is not anymore seen as a Hamiltonian acting on the Fock space but as a (self–adjoint) element of the CAR C^*–algebra $\mathcal{U}$ with thermodynamic phases describes by states on $\mathcal{U}$. Doing so we take advantage of the non–uniqueness of the representation of the CAR C^*–algebra $\mathcal{U}$. This property is indeed necessary to get non–unique equilibrium and ground states which imply phase transitions. This fact was first observed by R. Haag in 1962 [26], who established that the non–uniqueness of the ground state of the BCS model in infinite volume is related to the existence of several inequivalent[9] irreducible representations[10] of the Hamiltonian, see also [6, 27].

Equilibrium states define tangents to the convex map

$$\left(\beta,\mu,\lambda,\gamma,h\right)\mapsto\mathrm{p}\left(\beta,\mu,\lambda,\gamma,h\right).$$

The analysis of the set of tangents of this map gives hence information about the expectations of many important observables w.r.t. equilibrium states. The main technical point in the present work is therefore to find an explicit representation of the pressure by using the permutation invariance of the model in a crucial way. Indeed, we adapt to our case of fermions on a lattice the methods of [19] used to find the pressure of spin systems of mean–field type. Then, it is proven that it suffices to minimize the variational problem (1.5) w.r.t. the set $\mathcal{E}_{\mathcal{U}}^{S,+}$

[6] See Remark 6.1 in Section 6.1.

[7] The map $\omega\mapsto\mathfrak{F}(\omega)$ on the convex set $E_{\mathcal{U}}^{S,+}$ is affine and lower semicontinuous, thus Ω_β is a non empty face of $E_{\mathcal{U}}^{S,+}$.

[8] A face F of a compact convex set K is subset of K with the property that if $\omega=\Sigma_{n=1}^m\lambda_n\omega_n\in\mathrm{F}$ with $\Sigma_{n=1}^m\lambda_n=1$ and $\{\omega_n\}_{n=1}^m\subset\mathrm{K}$, then $\{\omega_n\}_{n=1}^m\subset\mathrm{F}$.

[9] This means that there is no isomorphism between $\mathfrak{h}_{j_1}$ and $\mathfrak{h}_{j_2}$ whenever $\mathfrak{h}_{j_1}$ and $\mathfrak{h}_{j_2}$ are the Hilbert spaces corresponding to two different irreducible representations.

[10] This means that the Hamiltonian can be seen as an operator acting on several Hilbert spaces $\{\mathfrak{h}_j\}_{j\in J}$ with no (non-trivial) invariant subspace.

of extremal states in $E_{\mathcal{U}}^{S,+}$. By adapting the proof of Størmer's theorem [1] to even states on the CAR algebra, we show next that extremal, permutation invariant and even states are product states

$$\omega_\zeta := \bigotimes_{x\in\mathbb{Z}^d} \zeta_x$$

obtained by "copying" some one–site even state ζ to all other sites. This result is a non–commutative version of the celebrated de Finetti Theorem from (classical) probability theory [28]. Using this, the variational problem (1.5) can be drastically simplified to a minimization problem on a finite dimensional manifold. At the end, it yields to another explicit, rather simple, variational problem on $\mathbb{R}_0^+$, which can be rigorously analyzed by analytic or numerical methods to obtain the complete thermodynamic behavior of the model.

Observe however, that all correlation functions *cannot* be drawn from an explicit formula for the pressure by taking derivatives combined with Griffiths arguments [29, 30, 31] on the convergence of derivatives of convex functions, unless the (infinite volume) pressure is shown to be differentiable w.r.t. any perturbation. Showing differentiability of the pressure as well as the explicit computation of its corresponding derivative can be a very hard task, for instance for correlation functions involving many lattice points. By contrast, the method presented in this paper gives access to all correlation functions at once. This is one basic (mathematical) message of this method, which is generalized in [18] to all translation invariant Fermi systems without requiring any quantum spin representation.

In fact, we precisely characterize the sets Ω_β for all $\beta \in (0,\infty]$, where Ω_∞ is the set of ground states with parameters μ, γ, λ, and h. This detailed study yields our main rigorous results on the strong coupling BCS–Hubbard model H_N, which can be summarized as follows:

- There is a set of parameters $\mathcal{S}$, defining the superconducting phase, with equilibrium and ground states breaking the $U(1)$–gauge symmetry and showing *off–diagonal long range order* (ODLRO).
- Depending on the parameters, the superconducting phase transition is either a first order or a second order phase transition.
- The superconducting phase $\mathcal{S}$ is characterized by the formation of Cooper pairs (shown by proving bounds for the density–density correlations) and a depleted Cooper pair condensate, the density $\mathrm{r}_\beta \in [0,1/4]$ of which is defined by the gap equation.
- From our proof of Størmer's theorem [1] for even states on the CAR algebra, we observe that the superconducting phase $\mathcal{S}$ corresponds to a *s–wave* superconductor, i.e., a superconductor with two–point correlation function, for $x,y\in\mathbb{Z}^d$, $s_1,s_2\in\{\uparrow,\downarrow\}$ and within $\mathcal{S}$, equal to $\omega(a_{x,s_1}a_{y,s_2}) = \mathrm{r}_\beta^{1/2}e^{i\phi}\neq 0$ if $x=y$ and $s_1\neq s_2$, and $\omega(a_{x,s_1}a_{y,s_2})=0$ else. (Here ω is any pure state of Ω_β; $\phi\in[0,2\pi)$ is determined by ω.)
- We observe the Meißner effect[11] by analyzing the relation between superconductivity and magnetization.
- We establish the existence of a superconductor–Mott insulator phase transition for integer electron density per site.
- The coexistence of ferromagnetic and superconducting phases is shown to be feasible at (critical) points of the boundary $\partial\mathcal{S}$ of $\mathcal{S}$, by applying the decomposition theory for states [32] on the weak*–compact and convex set Ω_β.
- The critical temperature θ_c for the superconducting phase transition w.r.t. λ, γ or h is analyzed in the case of fixed chemical potential μ and also in the case of constant electron density ρ. It shows that θ_c can be an *increasing* function of the *positive* coupling constant $\lambda>0$ at fixed $\mu\in\mathbb{R}$ but not at fixed $\rho>0$.
- For $\lambda\sim\gamma$ the critical temperature θ_c shows – as a function of the electron density ρ – the typical behavior observed (only) in high–T_c superconductors: θ_c is zero or very small for $\rho\sim 1$ and is much larger for ρ away from 1. Thus, our model provides a simple rigorous microscopic explanation for such experimentally well–known behavior of high–T_c superconductors.

[11] It is mathematically defined here by the absence of magnetization in presence of superconductivity. Steady surface currents around the bulk of the superconductor are not analyzed as it is a finite volume effect.

- Together with our study of the heat capacity, all these results can be used to fix experimentally all parameters of H_N.

Note that our study of equilibrium states is reminiscent of the work of Fannes, Spohn and Verbeure [33], performed however within a different framework. By opposition with our setting, their analysis [33] concerns symmetric states on an infinite tensor product of one C^*–algebra and their definition of equilibrium states uses the so–called correlation inequalities for KMS–states, see [29, Appendix E].

To conclude, this paper is organized as follows. In Section 2 we give the thermodynamic limit of the pressure p_N (1.4) as well as the gap equation. Then, our main results concerning the thermodynamic properties of the model are formulated in Section 3 at fixed chemical potential μ and in Section 4 at fixed electron density ρ per site. Section 5 briefly explains our result on the level of equilibrium states and gives additional remarks. In order to keep the main issues and the physical implications as transparent as possible, we reduce the technical and formal aspects to a minimum in Sections 2–5. In particular, in Sections 2–4 we only stay on the level of pressure and thermodynamic limit of local Gibbs states. The generalization of the results on the level of equilibrium and ground states is postponed to Section 6.2. Indeed, the rather long Section 6 gives the detailed mathematical foundations of our phase diagrams. In particular, in Section 6.1 we introduce the C^*–algebraic machinery needed in our analysis and prove various technical facts to conclude in Section 6.2 with the rigorous study of equilibrium and ground states. In Section 7, we collect some useful properties on the qualitative behavior of the Cooper pair condensate density, whereas Section 8 is an appendix on Griffiths arguments [29, 30, 31].

2. Grand–canonical pressure and gap equation

In order to obtain the thermodynamic behavior of the strong coupling BCS–Hubbard model H_N, it is essential to get first the thermodynamic limit $N \to \infty$ of its grand–canonical pressure p_N (1.4). The rigorous derivation of this limit is performed in Section 6.1. We explain here the final result with the heuristic behind it.

The first important remark is that one can guess the correct variational problem by the so-called approximating Hamiltonian method [34, 35, 36] originally proposed by Bogoliubov Jr. [37]. In our case, the correct approximation of the Hamiltonian H_N is the c–dependent Hamiltonian

$$
\begin{aligned}
H_N(c) := \quad & -\mu \sum_{x\in\Lambda_N} (n_{x,\uparrow} + n_{x,\downarrow}) - h \sum_{x\in\Lambda_N} (n_{x,\uparrow} - n_{x,\downarrow}) + 2\lambda \sum_{x\in\Lambda_N} n_{x,\uparrow} n_{x,\downarrow} \\
& -\frac{\gamma}{N} \sum_{x\in\Lambda_N} \left((Nc)\, a_{x,\uparrow}^* a_{x,\downarrow}^* + (N\bar{c})\, a_{x,\downarrow} a_{x,\uparrow} \right), \qquad (2.1)
\end{aligned}
$$

with $c \in \mathbb{C}$, see also [6, 7]. The main advantage of this Hamiltonian in comparison with H_N is the fact that it is a sum of shifts of the same local operator. For an appropriate order parameter $c \in \mathbb{C}$, it leads to a good approximation of the pressure p_N as $N \to \infty$. This can be partially seen from the inequality

$$
\gamma N |c|^2 + H_N(c) - \mathrm{H}_N = \frac{\gamma}{N} \left(\sum_{x\in\Lambda_N} a_{x,\uparrow}^* a_{x,\downarrow}^* - N\bar{c} \right) \left(\sum_{x\in\Lambda_N} a_{x,\uparrow} a_{x,\downarrow} - Nc \right) \geq 0,
$$

which is valid as soon as $\gamma \geq 0$. Observe that the constant term $\gamma N |c|^2$ is not included in the definition of $H_N(c)$. Hence, by using the Golden-Thompson inequality $\mathrm{Trace}(e^{A+B^*B}) \leq \mathrm{Trace}(e^A)$, the thermodynamic limit $\mathrm{p}(\beta,\mu,\lambda,\gamma,h)$ of the pressure p_N (1.4) is bounded from below by

$$
\mathrm{p}(\beta,\mu,\lambda,\gamma,h) \geq \sup_{c\in\mathbb{C}} \left\{ -\gamma|c|^2 + p(c) \right\}. \qquad (2.2)
$$

The function $p(c) = p(\beta,\mu,\lambda,\gamma,h;c)$ is the pressure associated with $H_N(c)$ for any $N \geq 1$. It can easily be computed since $H_N(c)$ is a sum of local operators which commute with each other. Indeed, for any $N \geq 1$, this pressure equals[12]

$$
\begin{aligned}
p(c) := \quad & \frac{1}{\beta N} \ln \mathrm{Trace}\left(e^{-\beta H_N(c)} \right) = \frac{1}{\beta} \ln \mathrm{Trace}\left(e^{-\beta H_1(c)} \right) \\
= \quad & \frac{1}{\beta} \ln \mathrm{Trace}\left(e^{\beta\left\{ (\mu+h) n_\uparrow + (\mu-h) n_\downarrow + \gamma(c a_\downarrow^* a_\uparrow^* + \bar{c} a_\uparrow a_\downarrow) - 2\lambda n_\uparrow n_\downarrow \right\}} \right). \qquad (2.3)
\end{aligned}
$$

[12]Here $a_{0,\uparrow}$, $a_{0,\downarrow}$ and $n_{0,\uparrow}$, $n_{0,\downarrow}$ are replaced respectively by $a_\uparrow$, $a_\downarrow$ and $n_\uparrow$, $n_\downarrow$.

To be useful, the variational problem in (2.2) should also be an upper bound of $\mathrm{p}(\beta,\mu,\lambda,\gamma,h)$. By adapting the proof of Størmer's theorem [1] to even states on the CAR algebra and by using the Petz–Raggio–Verbeure proof for spin systems [19] as a guideline, we prove this in Section 6.1. Thus, the thermodynamic limit of the pressure of the model H_N exists and can explicitly be computed by using the approximating Hamiltonian $H_N(c)$:

Theorem 2.1 (Grand-canonical pressure)
For any $\beta,\gamma>0$ and $\mu,\lambda,h\in\mathbb{R}$, the thermodynamic limit $\mathrm{p}(\beta,\mu,\lambda,\gamma,h)$ of the grand–canonical pressure p_N (1.4) equals

$$\mathrm{p}\left(\beta,\mu,\lambda,\gamma,h\right)=\sup_{c\in\mathbb{C}}\left\{-\gamma|c|^2+p\left(c\right)\right\}=\beta^{-1}\ln 2+\mu+\sup_{r\geq 0}f\left(r\right)<\infty,$$

where the real function $f\left(r\right)=f(\beta,\mu,\lambda,\gamma,h;r)$ is defined by

$$f\left(r\right):=-\gamma r+\frac{1}{\beta}\ln\left\{\cosh\left(\beta h\right)+e^{-\lambda\beta}\cosh\left(\beta g_r\right)\right\},$$

with $g_r:=\{(\mu-\lambda)^2+\gamma^2 r\}^{1/2}$.

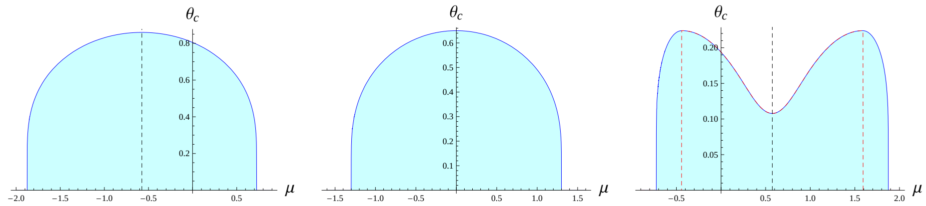

Figure 1: *Illustration, as a function of μ, of the critical temperature $\theta_c=\theta_c(\mu,\lambda,\gamma,h)$ such that $\mathrm{r}_\beta>0$ if and only if $\beta>\theta_c^{-1}$ (blue area) for $\gamma=2.6$, $h=0$ and with $\lambda=-0.575$ (left figure), 0 (figure on the center) and 0.575 (right figure). The blue line corresponds to a second order phase transition, whereas the red dashed line represents the domain of μ with a first order phase transition. The black dashed line is the chemical potential $\mu=\lambda$ corresponding to an electron density per site equal to 1, see Section 3.*

Remark 2.2 *The fact that the pressure p_N coincides as $N\to\infty$ with the variational problem given by the so-called approximating Hamiltonian (here $H_N(c)$) was previously proven via completely different methods in [34] for a large class of Hamiltonian (including H_N) with BCS–type interaction. However, as explained in the introduction, our proof gives deeper results, not expressed in Theorem 2.1, on the level of states, cf. (1.5) and (6.33). In contrast to the approximating Hamiltonian method [34, 35, 36, 37], it leads to a natural notion of equilibrium and ground states and allows the direct analysis of correlation functions. For more details, we recommend Section 6, particularly Section 6.2.*

From the gauge invariance of the map $c\mapsto p(c)$ observe that any maximizer $\mathrm{c}_\beta\in\mathbb{C}$ of the first variational problem given in Theorem 2.1 has the form $\mathrm{r}_\beta^{1/2}e^{i\phi}$ with $\mathrm{r}_\beta\geq 0$ being solution of

$$\sup_{r\geq 0}f(r)=f(\mathrm{r}_\beta) \tag{2.4}$$

and $\phi\in[0,2\pi)$. For any $\beta,\gamma>0$ and real numbers μ,λ,h, it is also clear that the order parameter r_β is always bounded since $f(r)$ diverges to $-\infty$ when $r\to\infty$. Up to (special) points $(\beta,\mu,\lambda,\gamma,h)$ corresponding to a phase transition of first order, it is always unique and continuous w.r.t. each parameter (see Section 7).

For low inverse temperatures β (high temperature regime) $\mathrm{r}_\beta=0$. Indeed, straightforward computations at low enough β show that the function $f(r)$ is concave as a function of $r\geq 0$ whereas $\partial_r f(0)<0$, see Section 7. On the other hand, any non–zero solution r_β of the variational problem (2.4) has to be solution of the gap equation (or Euler–Lagrange equation)

$$\tanh\left(\beta g_{\mathrm{r}_\beta}\right)=\frac{2g_{\mathrm{r}_\beta}}{\gamma}\left(1+\frac{e^{\lambda\beta}\cosh\left(\beta h\right)}{\cosh\left(\beta g_{\mathrm{r}_\beta}\right)}\right). \tag{2.5}$$

If $g_r = 0$, observe that one uses in (2.5) the asymptotics $x^{-1}\tanh x \sim 1$ as $x \to 0$, see also (7.2). Because $\tanh(x) \leq 1$ for $x \geq 0$, we then conclude that

$$0 \leq \mathrm{r}_\beta \leq \max\{0, \mathrm{r}_{\max}\}, \text{ with } \mathrm{r}_{\max} := \frac{1}{4} - \gamma^{-2}(\mu - \lambda)^2. \tag{2.6}$$

In particular, if $\gamma \leq 2|\mu - \lambda|$, then $\mathrm{r}_\beta = 0$ for any $\beta > 0$. However, at large enough $\beta > 0$ (low temperature regime) and at fixed $\lambda, h, \mu \in \mathbb{R}$, there is a unique $\gamma_c > 2|\lambda - \mu|$ such that $\mathrm{r}_\beta > 0$ for any $\gamma \geq \gamma_c$. In other words, the domain of parameters $(\beta, \mu, \lambda, \gamma, h)$ where r_β is strictly positive is non–empty, see figures 1–2 and Section 7. Observe in figure 2 that a positive λ, i.e., a one–site repulsion, can significantly increase (right figure) the critical temperature $\theta_c = \theta_c(\mu, \lambda, \gamma, h)$, which is defined such that $\mathrm{r}_\beta > 0$ if and only if $\beta > \theta_c^{-1}$.

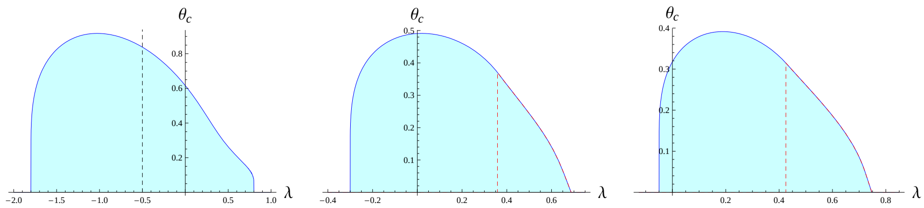

Figure 2: *Illustration, as a function of* λ*, of the critical temperature* $\theta_c = \theta_c(\mu, \lambda, \gamma, h)$ *for* $\gamma = 2.6$, $h = 0$ *and with* $\mu = -0.5$ *(left figure),* $\mu = 1$ *(figure at the center) and* $\mu = 1.25$ *(right figure). The blue line corresponds to a second order phase transition, whereas the red dashed line represents the domain of* λ *with first order phase transition. The black dashed line is the coupling constant* $\lambda = \mu$ *corresponding to an electron density per site equal to* 1*, see Section 3.*

From Lemma 7.1, the set of maximizers of the variational problem (2.4) has at most two elements in $[0, 1/4]$. It follows by continuity of $(\beta, \mu, \lambda, \gamma, h, r) \mapsto f(\beta, \mu, \lambda, \gamma, h; r)$, and from the fact that the interval $[0, 1/4]$ is compact, that the set

$$\mathcal{S} := \Big\{(\beta, \mu, \lambda, \gamma, h) \ : \ \beta, \gamma > 0 \text{ and } \mathrm{r}_\beta > 0 \text{ is the unique maximizer of (2.4)}\Big\} \tag{2.7}$$

is open. In Section 3.1, we prove that the set $\mathcal{S}$ corresponds to the superconducting phase since the order parameter solution of (2.4) can be interpreted as the Cooper pair condensate density. The boundary $\partial\mathcal{S}$ of the set $\mathcal{S}$ is called the set of *critical points* of our model. By definition, if (2.4) has more than one maximizer, then $(\beta, \mu, \lambda, \gamma, h) \in \partial\mathcal{S}$, whereas if $(\beta, \mu, \lambda, \gamma, h) \notin \overline{\mathcal{S}}$, then $r = 0$ is the unique maximizer of (2.4).

For more details on the study of the variational problem (2.4), we recommend Section 7.

3. Phase diagram at fixed chemical potential

By using our main theorem, i.e., Theorem 2.1, we can now explain the thermodynamic behavior of the strong coupling BCS–Hubbard model H_N. The rigorous proofs are however given in Section 6.2. Actually, we concentrate here on the physics of the model extracted from the (finite volume) grand–canonical Gibbs state ω_N (1.6) associated with H_N. We start by showing the existence of a superconducting phase transition in the thermodynamic limit.

3.1 Existence of a s–wave superconducting phase transition

The solution r_β of (2.4) can be interpreted as an order parameter related to the Cooper pair condensate density $\omega_N(\mathfrak{c}_0^*\mathfrak{c}_0)/N$, where

$$\mathfrak{c}_0 := \frac{1}{\sqrt{N}} \sum_{x \in \Lambda_N} a_{x,\downarrow} a_{x,\uparrow} = \frac{1}{\sqrt{N}} \sum_{k \in \Lambda_N^*} \tilde{a}_{k,\downarrow} \tilde{a}_{-k,\uparrow}$$

resp. $\mathfrak{c}_0^*$ annihilates resp. creates one Cooper pair within the condensate, i.e., in the zero-mode for electron pairs. Indeed, in Section 6.2 (see Theorem 6.13) we prove, by using a notion of equilibrium states, the following.

Theorem 3.1 (Cooper pair condensate density)
For any $\beta, \gamma > 0$ and real numbers μ, λ, h away from any critical point, the (infinite volume) Cooper pair condensate density equals

$$\begin{aligned}
\lim_{N\to\infty} \left\{ \frac{1}{N} \omega_N \left(\mathfrak{c}_0^* \mathfrak{c}_0 \right) \right\} &= \lim_{N\to\infty} \left\{ \frac{1}{N^2} \sum_{x,y\in\Lambda_N} \omega_N \left(a_{x,\uparrow}^* a_{x,\downarrow}^* a_{y,\downarrow} a_{y,\uparrow} \right) \right\} \\
&= \mathrm{r}_\beta \leq \max\left\{0, \mathrm{r}_{\max}\right\},
\end{aligned}$$

with $\mathrm{r}_{\max} \leq 1/4$ defined in (2.6). The (uniquely defined) order parameter $\mathrm{r}_\beta = \mathrm{r}_\beta(\mu, \lambda, \gamma, h)$ is an increasing function of $\gamma > 0$.

Remark 3.2 *In fact, Theorem 3.1 is not anymore satisfied only if the order parameter r_β is discontinuous w.r.t. $\gamma > 0$ at fixed (β, μ, λ, h). In this case, the thermodynamic limit of the Cooper pair condensate density is bounded by the left and right limits of the corresponding (infinite volume) density, see Section 8, in particular (8.1). Similar remarks can be done for Theorems 3.8, 3.10, 3.12 and 3.14.*

At least for large enough β and γ, we have explained that $\mathrm{r}_\beta > 0$, see figures 1–2. Illustrations of the Cooper pair condensate density r_β as a function of β and λ are given in figure 3. In other words, a superconducting phase transition can appear in our model. Its order depends on parameters: it can be a first order or a second order superconducting phase transition, cf. figure 3 and Section 7 for more details. From numerical investigations, note that r_β was always found to be an increasing function of $\beta > 0$. Unfortunately we are able to prove only a part of this fact in Section 7. Therefore, a superconducting phase appearing only in a range of non–zero temperatures as for magnetic superconductors cannot not rigorously been excluded. But we conjecture that our model can *never* show this phenomenon, i.e., r_β should always be an increasing function of $\beta > 0$.

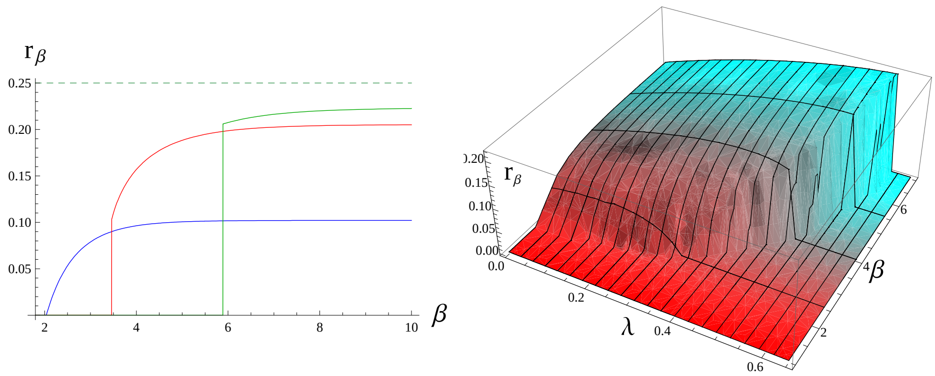

Figure 3: *In the figure on the left, we have three illustrations of the Cooper pair condensate density r_β as a function of the inverse temperature β for $\lambda = 0$ (blue line), $\lambda = 0.45$ (red line) and $\lambda = 0.575$ (green line). The figure on the right represents a 3D illustration of r_β as a function of λ and β. The color from red to blue reflects the decrease of the temperature. In all figures, $\mu = 1$, $\gamma = 2.6$ and $h = 0$.*

Observe that a non–trivial solution $\mathrm{r}_\beta \neq 0$ is a manifestation of the breakdown of the $U(1)$–gauge symmetry. To see this phenomenon, we need to perturb the Hamiltonian H_N with the external field

$$\alpha\sqrt{N}\left(e^{-i\phi}\mathfrak{c}_0 + e^{i\phi}\mathfrak{c}_0^*\right) \text{ for any } \alpha \geq 0 \text{ and } \phi \in [0, 2\pi).$$

This leads to the perturbed Gibbs state $\omega_{N,\alpha,\phi}(\cdot)$ defined by (1.6) with H_N replaced by

$$\mathrm{H}_{N,\alpha,\phi} := \mathrm{H}_N - \alpha \sum_{x\in\Lambda_N} \left(e^{-i\phi} a_{x,\downarrow} a_{x,\uparrow} + e^{i\phi} a_{x,\uparrow}^* a_{x,\downarrow}^* \right), \tag{3.1}$$

see (6.42). We then obtain the following result for the so–called Bogoliubov quasi–averages (cf. Theorem 6.12).

Theorem 3.3 (Breakdown of the $U(1)$-gauge symmetry)
For any $\beta, \gamma > 0$ and real numbers μ, λ, h away from any critical point, and for any $\phi \in [0, 2\pi)$, one gets for the Bogoliubov quasi–average below:

$$\lim_{\alpha \downarrow 0} \lim_{N \to \infty} \omega_{N,\alpha,\phi}(\mathfrak{c}_0/\sqrt{N}) = \lim_{\alpha \downarrow 0} \lim_{N \to \infty} \left\{ \frac{1}{N} \sum_{x \in \Lambda_N} \omega_{N,\alpha,\phi}\left(a_{x,\uparrow} a_{x,\downarrow}\right) \right\} = \mathrm{r}_\beta^{1/2} e^{i\phi},$$

with $\mathrm{r}_\beta \geq 0$ being the unique solution of (2.4), see Theorem 2.1.

Note that the breakdown of the $U(1)$–gauge symmetry should be "seen" in experiments via the so–called *off diagonal long range order* (ODLRO) property of the correlation functions [38], see Section 6.2. In fact, because of the permutation invariance, Theorem 3.1 still holds if we remove the space average, i.e., for any lattice sites x and $y \neq x$,

$$\lim_{N \to \infty} \omega_N(a_{y,\downarrow}^* a_{y,\uparrow}^* a_{x,\uparrow} a_{x,\downarrow}) = \mathrm{r}_\beta,$$

see Theorem 6.13. Similar remarks can be done for Theorems 3.8, 3.10, 3.12 and 3.14.

Observe also that the type of superconductivity described here is the *s–wave* superconductivity, which is defined via the two–point correlation function.

Theorem 3.4 (s–wave superconductivity)
For any $\beta, \gamma > 0$ and real numbers μ, λ, h away from any critical point, and for any $\phi \in [0, 2\pi)$, $x, y \in \mathbb{Z}^d$ and $s_1, s_2 \in \{\uparrow, \downarrow\}$, the two–point correlation function defined from the Bogoliubov quasi–averages equals

$$\lim_{\alpha \downarrow 0} \lim_{N \to \infty} \omega_{N,\alpha,\phi}(a_{x,s_1} a_{y,s_2}) = \mathrm{r}_\beta^{1/2} e^{i\phi} \delta_{x,y} \left(1 - \delta_{s_1,s_2}\right),$$

with $\mathrm{r}_\beta \geq 0$ being the unique solution of (2.4), see Theorem 2.1. Here $\delta_{x,y} = 1$ if and only if $x = y$.

In other words, for $x, y \in \mathbb{Z}^d$ and $s_1, s_2 \in \{\uparrow, \downarrow\}$ the two–point correlation function inside the superconducting phase is non–zero if and only if $x = y$ and $s_1 \neq s_2$. More generally, for any infinite volume equilibrium state ω, we have $\omega(a_{x,s_1} a_{y,s_2}) = \omega(a_{0,s_1} a_{0,s_2}) \delta_{x,y}$, see Section 6.

We conclude now this analysis by giving the zero–temperature limit $\beta \to \infty$ of the Cooper pair condensate density r_β proven in Section 7.

Corollary 3.5 (Cooper pair condensate density at zero–temperature)
The Cooper pair condensate density $\mathrm{r}_\infty = \mathrm{r}_\infty(\mu, \lambda, \gamma, h)$ is equal at zero–temperature to

$$\mathrm{r}_\infty := \lim_{\beta \to \infty} \mathrm{r}_\beta = \begin{cases} \mathrm{r}_{\max} & \text{for any } \gamma > \Gamma_{|\mu-\lambda|, \lambda+|h|} \\ 0 & \text{for any } \gamma < \Gamma_{|\mu-\lambda|, \lambda+|h|} \end{cases}$$

with $\mathrm{r}_{\max} \leq 1/4$ (cf. (2.6) and figure 4) and

$$\Gamma_{x,y} := 2\left(y + \left\{y^2 - x^2\right\}^{1/2}\right) \chi_{[0,y)}(x)\, \chi_{(0,\infty)}(y) + 2x \chi_{[y,\infty)}(x) \geq 0$$

be defined for any $x \in \mathbb{R}_+$ and $y \in \mathbb{R}$. Here $\chi_{\mathcal{K}}$ is the characteristic function of the set $\mathcal{K} \subset \mathbb{R}$.

Remark 3.6 *If $\gamma = \Gamma_{|\mu-\lambda|, \lambda+|h|}$, straightforward estimations show that the order parameter r_β converges to $\mathrm{r}_\infty = 0$, see Section 7. This special case is a critical point at sufficiently large β. We exclude it in our discussion since all thermodynamic limits of densities in Section 3 are performed away from any critical point, see for instance Theorem 3.1.*

The result of Corollary 3.5 is in accordance with Theorem 3.1 in the sense that the order parameter r_∞ is an increasing function of $\gamma \geq 0$. Observe also that

$$\sup_{\lambda \in \mathbb{R}} \left\{\mathrm{r}_\infty\left(\mu, \lambda, \gamma, h\right)\right\} = \mathrm{r}_\infty\left(\mu, \mu, \gamma, h\right) = \frac{1}{4}$$

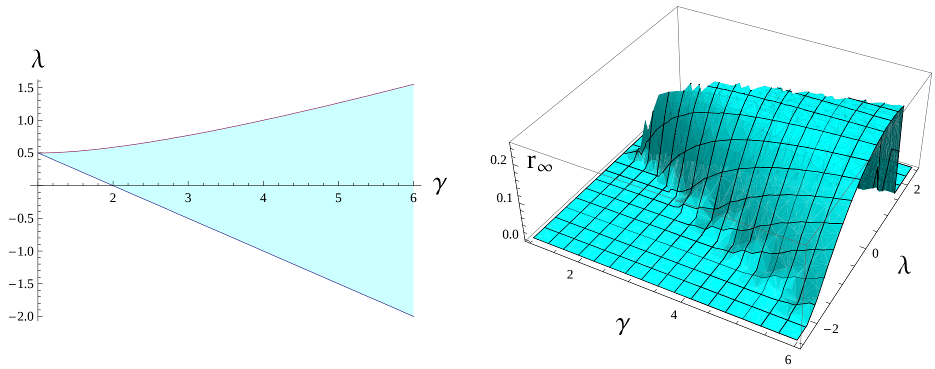

Figure 4: *In the figure on the left, the blue area represents the domain of* (λ, γ) *with* $1 \leq \gamma \leq 6$*, where the (zero–temperature) Cooper pair condensate density* r_∞ *is non–zero at* $\mu = 1$ *and* $h = 0$*. The figure on the right represents a 3D illustration of* r_∞ *when* $1 \leq \gamma \leq 6$ *and* $-2.5 \leq \lambda \leq 2.5$ *with again* $\mu = 1$, $h = 0$.

for any fixed $\gamma > \Gamma_{0,\mu+|h|}$, whereas for any real numbers μ, λ, h,

$$\lim_{\gamma \to \infty} \mathrm{r}_\infty (\mu, \lambda, \gamma, h) = \frac{1}{4}.$$

In other words, the superconducting phase for $\mu = \lambda$ is as perfect as for $\gamma = \infty$. In particular, in order to optimize the Cooper pair condensate density, if $\mu > 0$, then it is necessary to increase the one–site repulsion by tuning in λ to μ. Consequently, the direct repulsion between electrons can favor the superconductivity at fixed μ. This phenomenon is confirmed by the following analysis.

First observe that the equation (2.5) has no solution if $\gamma \leq 2|\mu|$ and $\lambda = 0$. In other words, the strong coupling BCS theory has no phase transition as soon as $\gamma \leq 2|\mu|$ and $\mu \neq 0$. However, even if $\gamma \leq 2|\mu|$, there is a range of λ where a superconducting phase takes place. For instance, take $\mu > 0$ and note that $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$ when

$$0 \leq \mu - \frac{\gamma}{2} < \lambda < \mu + \frac{\gamma}{2} - \sqrt{\gamma (\mu + |h|)}. \tag{3.2}$$

This last inequality can always be satisfied for some $\lambda > 0$, if $\mu + |h| < \gamma \leq 2\mu$. Therefore, although there is no superconductivity for $\gamma \leq 2|\mu|$ and $\lambda = 0$, there is a range of positive $\lambda \geq 0$ defined by (3.2) for $\mu + |h| < \gamma \leq 2\mu$, where the superconductivity appears at low enough temperature, see Corollary 3.5 and figure 4. In the region $\gamma \geq 2\mu > 0$ where the superconducting phase can occur for $\lambda = 0$, observe also that the critical temperature θ_c for $\lambda > 0$ can sometimes be larger as compared with the one for $\lambda = 0$, cf. figure 2.

Remark 3.7 *The effect of a one–site repulsion on the superconducting phase transition may be surprising since one would naively guess that any repulsion between pairs of electrons should destroy the formation of Cooper pairs. In fact, the one–site and BCS interactions in (1.2) are not diagonal in the same basis, i.e., they do not commute. In particular, the Hubbard interaction cannot be directly interpreted as a repulsion between Cooper pairs. This interpretation is only valid for large* $\lambda \geq 0$*. Indeed, at fixed* μ *and* $\gamma > 0$*, if* λ *is large enough, there is no superconducting phase.*

3.2 Electron density per site and electron–hole symmetry

We give next the grand–canonical density of electrons per site in the system (cf. Theorem 6.14).

Theorem 3.8 (Electron density per site)
For any $\beta, \gamma > 0$ *and real numbers* μ, λ, h *away from any critical point, the (infinite volume) electron density equals*

$$\lim_{N \to \infty} \left\{ \frac{1}{N} \sum_{x \in \Lambda_N} \omega_N (n_{x,\uparrow} + n_{x,\downarrow}) \right\} = \mathrm{d}_\beta := 1 + \frac{(\mu - \lambda) \sinh (\beta g_{\mathrm{r}_\beta})}{g_{\mathrm{r}_\beta} \left(e^{\beta\lambda} \cosh(\beta h) + \cosh (\beta g_{\mathrm{r}_\beta})\right)},$$

with $\mathrm{d}_\beta = \mathrm{d}_\beta(\mu, \lambda, \gamma, h) \in [0,2]$, $\mathrm{r}_\beta \geq 0$ *being the unique solution of (2.4) and* $g_r := \{(\mu-\lambda)^2 + \gamma^2 r\}^{1/2}$, *see Theorem 2.1 and figure 5.*

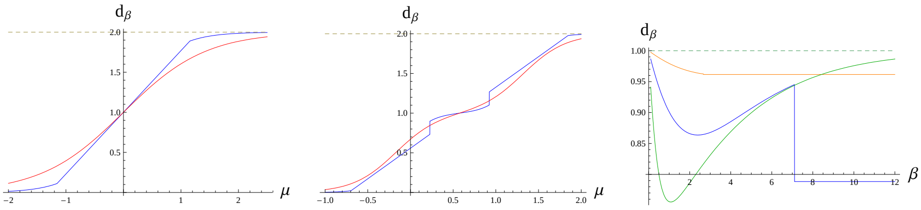

Figure 5: *In the figures on the left, we give illustrations of the electron density* d_β *as a function of the chemical potential* μ *for* $\beta < \beta_c$ *(red line) and* $\beta > \beta_c$ *(blue line) at coupling constant* $\lambda = 0$ *(figure on the left,* $\beta = 1.4$, 2.45*) and* $\lambda = 0.575$ *(figure on the center,* $\beta = 4$, 6.45*). In the figure on the right,* d_β *is given as a function of* β *at* $\mu = 0.3$ *with* $\lambda > \mu$ *equal to* 0.35 *(orange line, second order phase transition),* 0.575 *(blue line, first order phase transition) and* 1.575 *(green line, no phase transition). In all figures,* $\gamma = 2.6$, $h = 0$ *and* $\beta_c = \theta_c^{-1}$ *is the critical inverse temperature.*

At low enough temperature and for $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$, Corollary 3.5 tells us that a superconducting phase appears, i.e., $\mathrm{r}_\beta > 0$. In this case, it is important to note that the electron density becomes *independent* of the temperature. Indeed, by combining Theorem 3.8 with (2.5) one gets that

$$\mathrm{d}_\beta = 1 + 2\gamma^{-1}(\mu - \lambda) \tag{3.3}$$

is linear as a function of μ in the domain of $(\beta, \mu, \lambda, \gamma, h)$ where $\mathrm{r}_\beta > 0$, i.e., in the presence of superconductivity, see figure 5.

We give next the electron density per site in the zero–temperature limit $\beta \to \infty$, which straightforwardly follows from Theorem 3.8 combined with Corollary 3.5.

Corollary 3.9 (Electron density per site at zero–temperature)
The (infinite volume) electron density $\mathrm{d}_\infty = \mathrm{d}_\infty(\mu, \lambda, \gamma, h) \in [0,2]$ *at zero–temperature is equal to*

$$\mathrm{d}_\infty := \lim_{\beta\to\infty} \mathrm{d}_\beta = 1 + \frac{\mathrm{sgn}\,(\mu-\lambda)}{1 + \delta_{|\mu-\lambda|,\lambda+|h|}\,(1+\delta_{h,0})} \chi_{[\lambda+|h|,\infty)}\,(|\mu-\lambda|)$$

for $\gamma < \Gamma_{|\mu-\lambda|,\lambda+|h|}$*, whereas within the superconducting phase, i.e., for* $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$ *(Corollary 3.5),* $\mathrm{d}_\infty = 1 + 2\gamma^{-1}(\mu-\lambda)$*. Recall that* $\mathrm{sgn}(0) := 0$.

To conclude, observe that $(2 - \mathrm{d}_\beta)$ is the density of holes in the system. So, if $\mu > \lambda$, then $\mathrm{d}_\beta \in (1, 2]$, i.e., there are more electrons than holes in the system, whereas $\mathrm{d}_\beta \in [0, 1)$ for $\mu < \lambda$, i.e., there are more holes than electrons. This phenomenon can directly be seen in the Hamiltonian H_N, where there is a symmetry between electrons and holes as in the Hubbard model. Indeed, by replacing the creation operators $a^*_{x,\downarrow}$ and $a^*_{x,\uparrow}$ of electrons by the annihilation operators $-b_{x,\downarrow}$ and $-b_{x,\uparrow}$ of holes, we can map the Hamiltonian H_N (1.2) for electrons to another strong coupling BCS–Hubbard model for holes defined via the Hamiltonian

$$\begin{aligned}\widehat{H}_N \quad := \quad & -\mu_{\mathrm{hole}} \sum_{x\in\Lambda_N} (\hat{n}_{x,\uparrow} + \hat{n}_{x,\downarrow}) - h_{\mathrm{hole}} \sum_{x\in\Lambda_N} (\hat{n}_{x,\uparrow} - \hat{n}_{x,\downarrow}) + 2\lambda \sum_{x\in\Lambda_N} \hat{n}_{x,\uparrow}\hat{n}_{x,\downarrow} \\ & - \frac{\gamma}{N} \sum_{x,y\in\Lambda_N} b^*_{y,\uparrow} b^*_{y,\downarrow} b_{x,\downarrow} b_{x,\uparrow} + 2(\lambda-\mu)N - \gamma,\end{aligned}$$

with

$$\hat{n}_{x,\downarrow} := b^*_{x,\downarrow} b_{x,\downarrow},\ \hat{n}_{x,\uparrow} := b^*_{x,\uparrow} b_{x,\uparrow},\ h_{\mathrm{hole}} := -h \text{ and } \mu_{\mathrm{hole}} := 2\lambda - \mu - \gamma N^{-1}.$$

Therefore, if one knows the thermodynamic behavior of H_N for any $h \in \mathbb{R}$ and $\mu \geq \lambda$ (regime with more electrons than holes), we directly get the thermodynamic properties for $\mu < \lambda$ (regime with more holes than electrons), which correspond to the one given by $\widehat{H}_N$ with $h_{\mathrm{hole}} = -h$ and a chemical potential for holes $\mu_{\mathrm{hole}} > \lambda$ at large enough N. Note that the last constant term in $\widehat{H}_N$ shifts the grand–canonical pressure by a constant, but also the (infinite volume) mean–energy per site ϵ_β (Section 3.6).

3.3 Superconductivity versus magnetization: Meißner effect

It is well–known that for magnetic fields h with $|h|$ below some critical value $\mathrm{h}_\beta^{(c)}$, type I superconductors become perfectly diamagnetic in the sense that the magnetic induction in the bulk is zero. Magnetic fields with strength above $\mathrm{h}_\beta^{(c)}$ destroy the superconducting phase completely. This property is the celebrated Meißner or Meißner–Ochsenfeld effect. For small fields h (i.e., $|h| < \mathrm{h}_\beta^{(c)}$) the magnetic field in the bulk of the superconductor is (almost) cancelled by the presence of steady surface currents. As we do not analyze transport here, we only give the magnetization density explicitly as a function of the external magnetic field h for the strong coupling BCS–Hubbard model. Note that type II superconductors cannot be covered in the strong coupling regime since the vortices appearing in presence of magnetic fields come from the magnetic kinetic energy.

Theorem 3.10 (Magnetization density)
For any $\beta, \gamma > 0$ and real numbers μ, λ, h away from any critical point, the (infinite volume) magnetization density equals

$$\lim_{N\to\infty} \left\{ \frac{1}{N} \sum_{x\in\Lambda_N} \omega_N \left(n_{x,\uparrow} - n_{x,\downarrow} \right) \right\} = \mathrm{m}_\beta := \frac{\sinh(\beta h)\, e^{\lambda\beta}}{e^{\lambda\beta}\cosh(\beta h) + \cosh\left(\beta g_{\mathrm{r}_\beta}\right)},$$

with $\mathrm{m}_\beta = \mathrm{m}_\beta(\mu, \lambda, \gamma, h) \in [-1, 1]$, $\mathrm{r}_\beta \geq 0$ being the unique solution of (2.4) and $g_r := \{(\mu-\lambda)^2 + \gamma^2 r\}^{1/2}$, see Theorem 2.1 and figure 6.

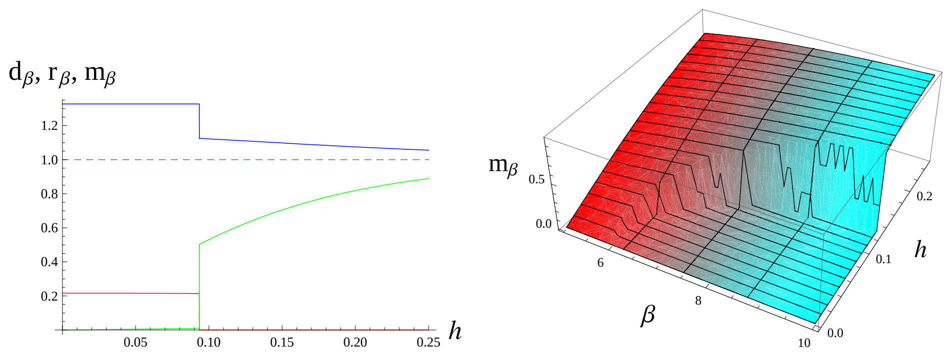

Figure 6: *In the figure on the left, we have an illustration of the electron density d_β (blue line), the Cooper pair condensate density r_β (red line) and the magnetization density m_β (green line) as functions of the magnetic field h at $\beta = 7$, $\mu = 1$, $\lambda = 0.575$ and $\gamma = 2.6$. The figure on the right represents a 3D illustration of $\mathrm{m}_\beta = \mathrm{m}_\beta(1, 0.575, 2.6, h)$ as a function of h and β. The color from red to blue reflects the decrease of the temperature. In both figures, we can see the Meißner effect (In the 3D illustration, the area with no magnetization corresponds to $\mathrm{r}_\beta > 0$).*

This theorem deduced from Theorem 6.14 does not seem to show any Meißner effect since $\mathrm{m}_\beta > 0$ as soon as $h \neq 0$. However, when the Cooper pair condensate density r_β is strictly positive, from Theorem 3.10 combined with (2.5) note that

$$\mathrm{m}_\beta = \frac{2 g_{\mathrm{r}_\beta} e^{\lambda\beta} \sinh(\beta h)}{\gamma \sinh\left(\beta g_{\mathrm{r}_\beta}\right)}. \tag{3.4}$$

In particular, it decays exponentially as $\beta \to \infty$ when $\mathrm{r}_\beta \to \mathrm{r}_\infty > 0$, see figure 6. We give therefore the zero–temperature limit $\beta \to \infty$ of m_β in the next corollary.

Corollary 3.11 (Magnetization density at zero–temperature)
The (infinite volume) magnetization density $\mathrm{m}_\infty = \mathrm{m}_\infty(\mu, \lambda, \gamma, h) \in [-1, 1]$ *at zero–temperature is equal to*

$$\mathrm{m}_\infty := \lim_{\beta\to\infty} \mathrm{m}_\beta = \frac{\mathrm{sgn}(h)}{1+\delta_{|\mu-\lambda|,\lambda+|h|}} \chi_{[0,\lambda+|h|]} (|\mu - \lambda|) ,$$

for $\gamma < \Gamma_{|\mu-\lambda|,\lambda+|h|}$ *(see Corollary 3.5), whereas for* $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$ *there is no magnetization at zero–temperature since* m_β *decays exponentially*[13] *as* $\beta \to \infty$ *to* $\mathrm{m}_\infty = 0$.

Consequently, there is no superconductivity, i.e. $\mathrm{r}_\infty = 0$, when $\gamma < \Gamma_{|\mu-\lambda|,\lambda+|h|}$ and, as soon as $h \neq 0$ with $|\mu - \lambda| < \lambda + |h|$, there is a perfect magnetization at zero–temperature, i.e., $\mathrm{m}_\infty = \mathrm{sgn}(h)$. Observe that the condition $|\mu - \lambda| > \lambda + |h|$ implies from Corollary 3.9 that either $\mathrm{d}_\infty = 0$ or $\mathrm{d}_\infty = 2$, which implies that m_∞ must be zero.

On the other hand, if $\gamma > \Gamma_{|\mu-\lambda|,\lambda}$, we can define the critical magnetic field at zero–temperature by the unique positive solution

$$\mathrm{h}_\infty^{(c)} := \gamma \left(\frac{1}{4} + \gamma^{-2} (\mu - \lambda)^2 \right) - \lambda > 0 \tag{3.5}$$

of the equation $\Gamma_{|\mu-\lambda|,\lambda+y} = \gamma$ for $y \geq 0$. Then, by increasing $|h|$ up to $\mathrm{h}_\infty^{(c)}$, the (zero–temperature) Cooper pair condensate density r_∞ stays constant, whereas the (zero–temperature) magnetization density m_∞ is zero, i.e., $\mathrm{r}_\infty = \mathrm{r}_{\max}$ and $\mathrm{m}_\infty = 0$ for $|h| < \mathrm{h}_\infty^{(c)}$, see Corollary 3.5. However, as soon as $|h| > \mathrm{h}_\infty^{(c)}$, $\mathrm{r}_\infty = 0$ and $\mathrm{m}_\infty = \mathrm{sgn}(h)$, i.e., there is no Cooper pair and a pure magnetization takes place. In other words, the model manifests a pure Meißner effect at zero–temperature corresponding to a superconductor of type I, cf. figure 6.

Finally, note that we give an energetic interpretation of the critical magnetic field $\mathrm{h}_\infty^{(c)}$ after Corollary 3.15. Observe also that a measurement of $\mathrm{h}_\infty^{(c)}$ (3.5) implies, for instance, a measurement of the chemical potential μ if one would know γ and λ, which could be found via the asymptotic (3.15) of the specific heat, see discussions in Section 5.

3.4 Coulomb correlation density

The space distribution of electrons is still unknown and for such a consideration, we need the (infinite volume) Coulomb correlation density

$$\lim_{N\to\infty} \left\{ \frac{1}{N} \sum_{x\in\Lambda_N} \omega_N (n_{x,\uparrow} n_{x,\downarrow}) \right\} . \tag{3.6}$$

Together with the electron and magnetization densities d_β and m_β, the knowledge of (3.6) allows us in particular to explain in detail the difference between superconducting and non–superconducting phases in terms of space distributions of electrons.

Actually, by the Cauchy–Schwarz inequality for the states one gets that

$$\frac{1}{N} \sum_{x\in\Lambda_N} \omega_N (n_{x,\uparrow} n_{x,\downarrow}) \leq \sqrt{\frac{1}{N} \sum_{x\in\Lambda_N} \omega_N (n_{x,\uparrow})} \sqrt{\frac{1}{N} \sum_{x\in\Lambda_N} \omega_N (n_{x,\downarrow})}. \tag{3.7}$$

From Theorems 3.8 and 3.10, the densities of electrons with spin up $\uparrow$ and down $\downarrow$ equal respectively

$$\lim_{N\to\infty} \left\{ \frac{1}{N} \sum_{x\in\Lambda_N} \omega_N (n_{x,\uparrow}) \right\} = \frac{\mathrm{d}_\beta + \mathrm{m}_\beta}{2} \in [0, 1]$$

and

$$\lim_{N\to\infty} \left\{ \frac{1}{N} \sum_{x\in\Lambda_N} \omega_N (n_{x,\downarrow}) \right\} = \frac{\mathrm{d}_\beta - \mathrm{m}_\beta}{2} \in [0, 1]$$

[13] Actually, $\mathrm{m}_\beta = \mathcal{O}(e^{-(\gamma-2(\lambda+|h|))\beta/2})$ for $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|} \geq 2(\lambda + |h|)$.

for any $\beta, \gamma > 0$ and μ, λ, h away from any critical point. Consequently, by using (3.7) in the thermodynamic limit, the (infinite volume) Coulomb correlation density is always bounded by

$$0 \leq \lim_{N\rightarrow\infty} \left\{ \frac{1}{N} \sum_{x\in\Lambda_N} \omega_N \left(n_{x,\uparrow} n_{x,\downarrow} \right) \right\} \leq \mathrm{w}_{\max} := \frac{1}{2}\sqrt{\mathrm{d}_\beta^2 - \mathrm{m}_\beta^2}. \tag{3.8}$$

If for instance (3.6) equals zero, then as soon as an electron is on a definite site, the probability to have a second electron with opposite spin at the same place goes to zero as $N \rightarrow \infty$. In this case, there would be no formation of pairs of electrons on a single site. This phenomenon does not appear exactly in finite temperature due to thermal fluctuations. Indeed, we can explicitly compute the Coulomb correlation in the thermodynamic limit (cf. Theorem 6.14):

Theorem 3.12 (Coulomb correlation density)
For any $\beta, \gamma > 0$ and real numbers μ, λ, h away from any critical point, the (infinite volume) Coulomb correlation density equals[14]

$$\lim_{N\rightarrow\infty} \left\{ \frac{1}{N} \sum_{x\in\Lambda_N} \omega_N \left(n_{x,\uparrow} n_{x,\downarrow} \right) \right\} = \mathrm{w}_\beta := \frac{1}{2} \left(\mathrm{d}_\beta - \mathrm{m}_\beta \coth \left(\beta h \right) \right),$$

with $\mathrm{w}_\beta = \mathrm{w}_\beta(\mu, \lambda, \gamma, h) \in (0, \mathrm{w}_{\max})$, see figure 7. Here d_β and m_β are respectively defined in Theorems 3.8 and 3.10.

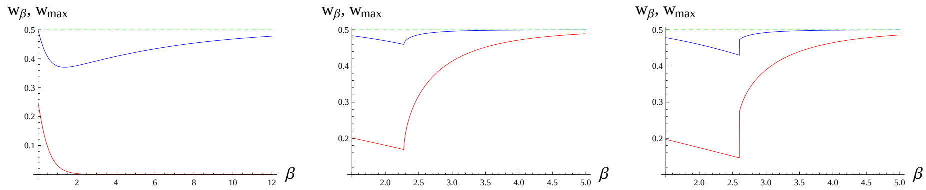

Figure 7: *Illustration of the Coulomb correlation density w_β (red lines) and its corresponding upper bound $\mathrm{w}_{\max}$ (blue lines) as a function of $\beta > 0$ at $\mu = 0.2$, $\gamma = 2.6$, for $\lambda = 1.305 < \mu$ (left figure, $\mathrm{d}_\beta < 1$), $\lambda = 0.2 = \mu$ (two right figures, $\mathrm{d}_\beta = 1$), and from the left to the right, with $h = 0$ ($\mathrm{m}_\beta = 0$), and $h = 0.3$, 0.35 (where $\mathrm{m}_\beta > 0$). The dashed green lines indicate that $\mathrm{d}_\infty/2 = 0.5$ in the three cases. In the figure on the left there is no superconducting phase in opposition to the right figures where we see a phase transition for $\beta > 2.3$ (second order) or 2.6 (first order).*

Consequently, because $g_{\mathrm{r}_\beta} \geq |\lambda - \mu|$, for any inverse temperature $\beta > 0$ the Coulomb correlation density is never zero, i.e., $\mathrm{w}_\beta > 0$, even if the electron density d_β is exactly 1, i.e., if $\lambda = \mu$. Moreover, the upper bound in (3.8) is also never attained. However, for low temperatures, w_β goes exponentially fast w.r.t. β to one of the bounds in (3.8), cf. figure 7. Indeed, one has the following zero–temperature limit:

Corollary 3.13 (Coulomb correlation density at zero–temperature)
The (infinite volume) Coulomb correlation density $\mathrm{w}_\infty = \mathrm{w}_\infty(\mu, \lambda, \gamma, h) \in [0, 1]$ at zero–temperature is equal to

$$\mathrm{w}_\infty := \lim_{\beta\rightarrow\infty} \mathrm{w}_\beta = \frac{1 + \mathrm{sgn}\left(\mu - \lambda\right)}{2\left(1 + \delta_{|\mu-\lambda|,\lambda+|h|}\left(1 + \delta_{h,0}\right)\right)} \chi_{[\lambda+|h|,\infty)}\left(|\mu - \lambda|\right)$$

for $\gamma < \Gamma_{|\mu-\lambda|,\lambda+|h|}$ whereas $\mathrm{w}_\infty = \mathrm{d}_\infty/2$ for $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$, see Corollaries 3.5-3.9.

If $|\mu - \lambda| > \lambda + |h|$, the interpretation of this asymptotics is clear since either $\mathrm{d}_\infty = 0$ for $\mu < \lambda$ or $\mathrm{d}_\infty = 2$ for $\mu > \lambda$. The interesting phenomena are when $|\mu - \lambda| < \lambda + |h|$. In this case, if there is no superconducting phase, i.e., $\gamma < \Gamma_{|\mu-\lambda|,\lambda+|h|}$, then w_β converges towards $\mathrm{w}_\infty = 0$ as $\beta \rightarrow \infty$. In particular, as explained above,

[14] If $h = 0$, then $\mathrm{w}_\beta(\mu, \lambda, \gamma, 0) := \lim_{h\rightarrow 0} \mathrm{w}_\beta(\mu, \lambda, \gamma, h)$.

if an electron is on a definite site, the probability to have a second electron with opposite spin at the same place goes to zero as $N \to \infty$ and $\beta \to \infty$.

However, in the superconducting phase, i.e., for $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$, the upper bound $\mathrm{w}_{\max}$ (3.8) is asymptotically attained. Since $\mathrm{w}_{\max} = \mathrm{d}_\infty/2$ as $\beta \to \infty$, it means that 100% of electrons form Cooper pairs in the limit of zero–temperature, which is in accordance with the fact that the magnetization density must disappear, i.e., $\mathrm{m}_\infty = 0$, cf. Corollary 3.11. As explained in Section 3.1, the highest Cooper pair condensate density is 1/4, which corresponds to an electron density $\mathrm{d}_\infty = 1$. Actually, although all electrons form Cooper pairs at small temperatures, there are never 100% of electron pairs in the condensate, see figure 8. In the special case where $\mathrm{d}_\infty = 1$, only 50% of Cooper pairs are in the condensate.

The same analysis can be done for hole pairs by changing a_x by $-b_x^*$ in the definition of extensive quantities. Define the electron and hole pair condensate fractions respectively by $\mathrm{v}_\beta := 2\mathrm{r}_\beta/\mathrm{d}_\beta$ and $\hat{\mathrm{v}}_\beta := 2\hat{\mathrm{r}}_\beta/\hat{\mathrm{d}}_\beta$, where $\hat{\mathrm{r}}_\beta$ and $\hat{\mathrm{d}}_\beta$ are the hole condensate density and the hole density respectively. Because of the electron–hole symmetry, $\hat{\mathrm{r}}_\beta = \mathrm{r}_\beta$ and $\hat{\mathrm{d}}_\beta = 2 - \mathrm{d}_\beta$. In particular, when $\mathrm{r}_\beta > 0$, we asymptotically get that $\hat{\mathrm{v}}_\beta + \mathrm{v}_\beta \to 1$ as $\beta \to \infty$. Hence, in the superconducting phase, an electron pair condensate fraction below 50% means in fact that there are more than 50% of hole pair condensate and conversely at low temperatures. For more details concerning ground states in relation with this phenomenon, see discussions around (6.60) in Section 6.2.

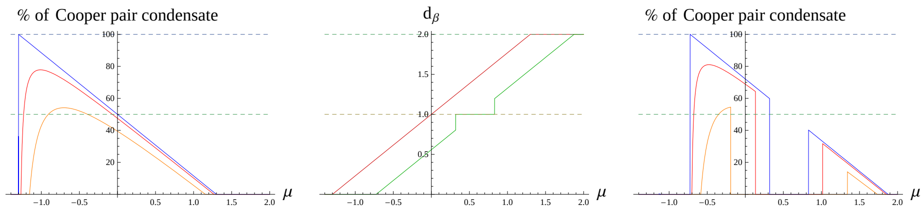

Figure 8: *The fraction of electron pairs in the condensate is given in right and left figures as a function of μ. In the figure on the left, $\lambda = h = 0$, with inverse temperatures $\beta = 2.45$ (orange line), 3.45 (red line) and 30 (blue line). In the figure on the right, $\lambda = 0.575$ and $h = 0.1$ with $\beta = 5$ (orange line), 7 (red line) and 30 (blue line). The figure on the center illustrates the electron density d_β also as a function of μ at $\beta = 30$ (low temperature regime) for $\lambda = h = 0$ (red line) and for $\lambda = 0.575$ and $h = 0.1$ (green line). In all figures, $\gamma = 2.6$.*

3.5 Superconductor–Mott insulator phase transition

By Corollary 3.9, if $\lambda > 0$ and the system is not in the superconducting phase (i.e., if $r_\beta = 0$), then the electron density converges to either 0, 1 or 2 as $\beta \to \infty$ since

$$\mathrm{d}_\infty = 1 + \mathrm{sgn}\,(\mu - \lambda)\,. \tag{3.9}$$

We define the phase where the system does not form a pair condensate and the electron density is around 1, as a *Mott insulator* phase. More precisely, we say that the system forms a Mott insulator, if for some $\epsilon < 1$, some $0 < \beta_0 < \infty$, some $\mu_0 \in \mathbb{R}$ and some $\delta\mu > 0$, the electron density

$$\mathrm{d}_\beta \in (1-\epsilon, 1+\epsilon) \text{ and } \mathrm{r}_\beta = 0 \text{ for all } (\beta,\mu) \in (\beta_0,\infty) \times (\mu_0 - \delta\mu, \mu_0 + \delta\mu).$$

As discussed in Section 3.4, observe that we have, in this phase, exactly one electron (or hole) localized in each site at the low temperature limit since $\mathrm{d}_\beta \to 1$ and $\mathrm{w}_\beta \to 0$ as $\beta \to \infty$.

To extract the whole region of parameters where such a thermodynamic phase takes place, a preliminary analysis of the function $\Gamma_{x,y}$ defined in Corollary 3.5 is first required. Observe that $\Gamma_{0,y} > 0$ if and only if $y > 0$. Consequently, for any real numbers λ and h such that $\lambda + |h| \leq 0$ we have $\Gamma_{0,\lambda+|h|} = 0$. However, if $\lambda + |h| > 0$ then $\Gamma_{0,\lambda+|h|} > 0$. Meanwhile, at fixed $y > 0$, the continuous function $\Gamma_{x,y}$ of $x \geq 0$ is convex with minimum for $x = y$, i.e.,

$$\inf_{x\geq 0} \{\Gamma_{x,y}\} = \Gamma_{y,y} = 2y > 0. \tag{3.10}$$

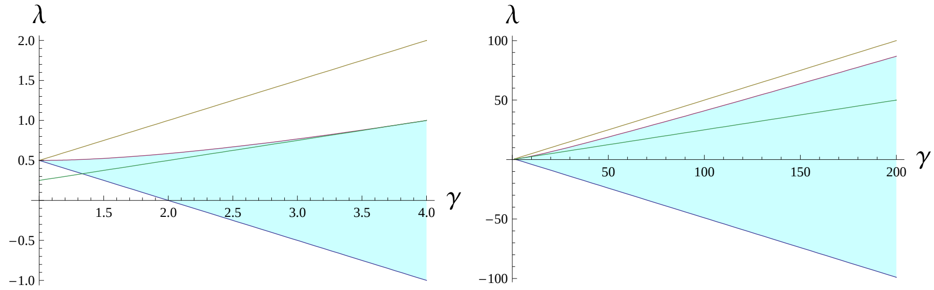

Figure 9: *In both figures, the blue area represents the domain of* (λ, γ)*, where there is a superconducting phase at zero temperature for* $\mu = 1$ *and* $h = 0$*. The two increasing straight lines (green and brown) are* $\gamma = 4\lambda$ *and* $\gamma = 2\lambda$ *for* $\gamma \geq 1$*. In particular, between these two lines* $(2\lambda < \gamma < 4\lambda)$*, there is a superconducting-Mott-Insulator phase transition by tuning* μ*.*

In particular, $\Gamma_{x,y}$ is strictly decreasing as a function of $x \in [0, y]$ and strictly increasing for $x \geq y$.

Now, by combining Corollaries 3.5, 3.9, 3.11 and 3.13, we are in position to extract the set of parameters corresponding to insulating or superconducting phases:

1. For any $\gamma > 0$ and $\mu, \lambda \in \mathbb{R}$ such that

$$|\mu - \lambda| > \max\{\gamma/2, \lambda + |h|\},$$

observe first that there are no superconductivity ($\mathrm{r}_\infty = 0$), either no electrons or no holes (see (3.9)) and, in any case, no magnetization since $\mathrm{m}_\infty = 0$. It is a standard (non ferromagnetic) insulator.

The next step is now to analyze the thermodynamic behavior for

$$|\mu - \lambda| < \max\{\gamma/2, \lambda + |h|\}, \tag{3.11}$$

which depends on the strength of $\gamma > 0$. From **2.** to **4.**, we assume that (3.11) is satisfied.

2. If the BCS coupling constant γ satisfies

$$0 < \gamma \leq \Gamma_{\lambda+|h|,\lambda+|h|} = 2(\lambda + |h|),$$

then from (3.10) combined with Corollary 3.5 there is no Cooper pair for any μ and any λ. In particular, under the condition (3.11) there are a perfect magnetization, i.e., $\mathrm{m}_\infty = \mathrm{sgn}(h)$, and exactly one electron or one hole per site since $\mathrm{d}_\infty = 1$ and $\mathrm{w}_\infty = 0$. In other words, we obtain a ferromagnetic Mott insulator phase.

3. Now, if $\gamma > 0$ becomes too strong, i.e.,

$$\gamma > \Gamma_{0,\lambda+|h|} = 4(\lambda + |h|),$$

then for any $\mu \in \mathbb{R}$ such that $|\mu - \lambda| < \gamma/2$ there are Cooper pairs because $\mathrm{r}_\infty = \mathrm{r}_{\max} > 0$, an electron density d_∞ equal to (3.3) and no magnetization ($\mathrm{m}_\infty = 0$). In this case, observe that all quantities are continuous at $|\mu - \lambda| = \gamma/2$. This is a superconducting phase.

4. The superconducting–Mott insulator phase transition only appears in the intermediary regime where

$$\Gamma_{\lambda+|h|,\lambda+|h|} = 2\,(\lambda + |h|) < \gamma < \Gamma_{0,\lambda+|h|} = 4\,(\lambda + |h|)\,, \tag{3.12}$$

cf. figure 9. Indeed, the function $\Gamma_{x,\lambda+|h|} = \gamma$ has two solutions

$$\mathrm{x}_1 := \frac{\gamma^{1/2}}{2}\{4\,(\lambda + |h|) - \gamma\}^{1/2} \text{ and } \mathrm{x}_2 := \frac{\gamma}{2} > \mathrm{x}_1.$$

In particular, for any $\mu \in \mathbb{R}$ such that $|\mu - \lambda| \in (\mathrm{x}_1, \gamma/2)$, the BCS coupling constant γ is strong enough to imply the superconductivity ($\mathrm{r}_\infty = \mathrm{r}_{\max} > 0$), with an electron density d_∞ equal to (3.3) and no magnetization ($\mathrm{m}_\infty = 0$). We are in the superconducting phase. However, for any $\mu \in \mathbb{R}$ such that $|\mu - \lambda| < \mathrm{x}_1$, the BCS coupling constant γ becomes too weak and there is no superconductivity ($\mathrm{r}_\infty = 0$), exactly one electron per site, i.e., $\mathrm{d}_\infty = 1$ and $\mathrm{w}_\infty = 0$, and a pure magnetization if $h \neq 0$, i.e., $\mathrm{m}_\infty = \mathrm{sgn}(h)$. In this regime, one gets a ferromagnetic Mott insulator phase. All quantities are continuous at $|\mu - \lambda| = \gamma/2$ but not for $|\mu - \lambda| = \mathrm{x}_1$. In other words, we get a superconductor–Mott insulator phase transition by tuning in the chemical potential μ. An illustration of this phase transition is given in figure 10, see also figure 8.

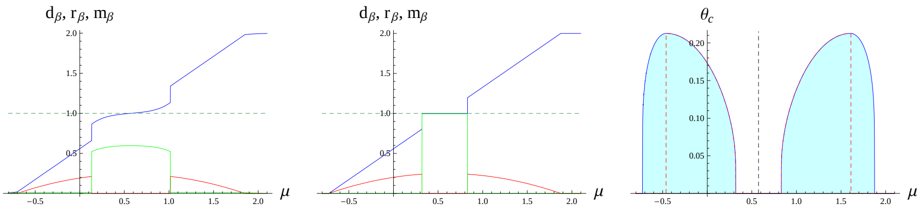

Figure 10: *Here* $\lambda = 0.575$, $\gamma = 2.6$, *and* $h = 0.1$. *In the two figures on the left, we plot the electron density* d_β *(blue line), the Cooper pair condensate density* r_β *(red line) and the magnetization density* m_β *(green line) as functions of* μ *for* $\beta = 7$ *(left figure) or* 30 *(low temperature regime, figure on the center). Observe the superconducting-Mott Insulator phase transition which appears in both cases. In the right figure, we illustrate as a function of* μ *the corresponding critical temperature* θ_c. *The blue line corresponds to a second order phase transition, whereas the red dashed line represents the domain of* μ *with first order phase transition. The black dashed line is the chemical potential* $\mu = \lambda$ *corresponding to an electron density per site equal to* 1.

3.6 Mean–energy per site and the specific heat

To conclude, low–T_c superconductors and high–T_c superconductors differ by the behavior of their specific heat. The first one shows a discontinuity of the specific heat at the critical point whereas the specific heat for high–T_c superconductors is continuous. It is therefore interesting to give now the mean–energy per site in the thermodynamic limit in order to compute next the specific heat.

Theorem 3.14 (Mean-energy per site)
For any $\beta, \gamma > 0$ *and real numbers* μ, λ, h *away from any critical point, the (infinite volume) mean energy per site is equal to*

$$\lim_{N\to\infty} \left\{ N^{-1} \omega_N \left(\mathrm{H}_N\right) \right\} = \epsilon_\beta := -\mu \mathrm{d}_\beta - h \mathrm{m}_\beta + 2\lambda \mathrm{w}_\beta - \gamma \mathrm{r}_\beta,$$

see Theorems 3.1, 3.8, 3.10, 3.12 and figure 11.

At zero–temperature, Corollaries 3.5, 3.9, 3.11 and 3.13 imply an explicit computation of the mean energy per site:

Corollary 3.15 (Mean-energy per site at zero–temperature)
The (infinite volume) mean energy per site $\epsilon_\infty = \epsilon_\infty(\mu, \lambda, \gamma, h)$ *at zero–temperature is equal to*

$$\begin{aligned} \epsilon_\infty \quad := \quad & \lim_{\beta\to\infty} \epsilon_\beta = -\mu + \frac{\lambda + |\lambda - \mu|}{1 + \delta_{|\mu-\lambda|,\lambda+|h|} \left(1 + \delta_{h,0}\right)} \chi_{[\lambda+|h|,\infty)} \left(|\mu - \lambda|\right) \\ & - \frac{|h|}{1 + \delta_{|\mu-\lambda|,\lambda+|h|}} \chi_{[0,\lambda+|h|]} \left(|\mu - \lambda|\right), \end{aligned}$$

for $\gamma < \Gamma_{|\mu-\lambda|,\lambda+|h|}$ *whereas for* $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$

$$\epsilon_\infty := \lim_{\beta\to\infty} \epsilon_\beta = -\frac{\gamma}{4} + (\lambda - \mu) \left(1 + \gamma^{-1} (\mu - \lambda)\right),$$

cf. Corollary 3.5.

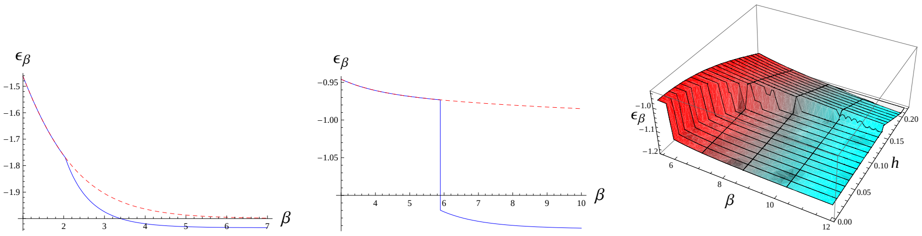

Figure 11: *In the two figures on the left, we give the mean energy per site ϵ_β as a function of β at $h = 0$ for $\lambda = 0$ (figure on the left, second order BCS phase transition) or $\lambda = 0.575$ (figure on the center, first order phase transition). The dashed line in both figures is the mean energy per site with zero Cooper pair condensate density. On the right figure, ϵ_β is given as a function of β and h at $\lambda = 0.575$. The color from red to blue reflects the decrease of the temperature and the plateau corresponds to the superconducting phase. In all figures, $\mu = 1$ and $\gamma = 2.6$.*

Note that the critical magnetic field $\mathrm{h}_\infty^{(c)}$ (3.5) has a direct interpretation in terms of the zero–temperature mean energy per site ϵ_∞. Indeed, if $|\mu - \lambda| < \lambda + |h|$, i.e., $\mathrm{d}_\infty \notin \{0, 2\}$, by equating ϵ_∞ in the superconducting phase with the mean energy $\epsilon_\infty = -\mu - |h|$ in the non–superconducting (ferromagnetic) state, we directly get that the magnetic field should be equal to $|h| = \mathrm{h}_\infty^{(c)}$ (3.5). In other words, the critical magnetic field $\mathrm{h}_\infty^{(c)}$ corresponds to the point where the mean energies at zero-temperature in both cases are equal to each other, as it should be. Note that this phenomenon is not true at non–zero temperature since the mean energy per site can be discontinuous as a function of h (even if $\lambda = 0$), see figure 11.

Now, the specific heat at finite volume equals

$$\mathrm{c}_{N,\beta} := -\beta^2 \partial_\beta \left\{ N^{-1} \omega_N \left(\mathrm{H}_N \right) \right\} = N^{-1} \beta^2 \omega_N \left(\left[\mathrm{H}_N - \omega_N \left(\mathrm{H}_N \right) \right]^2 \right). \tag{3.13}$$

However, its thermodynamic limit

$$\mathrm{c}_\beta := \lim_{N \to \infty} \mathrm{c}_{N,\beta} = -\beta^2 \partial_\beta \epsilon_\beta + \mathfrak{C}_\beta \tag{3.14}$$

cannot be easily computed because one cannot exchange the limit $N \to \infty$ and the derivative ∂_β, i.e., $\mathfrak{C}_\beta = \mathfrak{C}_\beta(\mu, \lambda, \gamma, h)$ may be non–zero. For instance, Griffiths arguments [29, 30, 31] (Section 8) would allow to exchange any derivative of the pressure p_N and the limit $N \to \infty$ by using the convexity of p_N. To compute (3.14) in this way, we would need to prove the (piece–wise) convexity of $\epsilon_{N,\beta} := N^{-1} \omega_N \left(\mathrm{H}_N \right)$ as a function $\beta > 0$. As suggested by figure 11, this property of convexity might be right but it is not proven here.

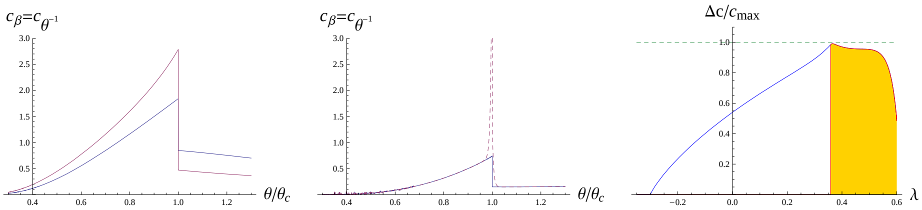

Figure 12: *Here $\mu = 1$, $\gamma = 2.6$ and $h = 0$. Assuming $\mathfrak{C}_\beta = 0$, we give 3 plots of the specific heat c_β as a function of the ratio θ/θ_c between $\theta := \beta^{-1}$ and the critical temperature θ_c for $\lambda = 0$, 0.5 (both left figure, respectively blue and red lines, second order phase transition), and $\lambda = 0.575$ (figure on the center, blue line, first order phase transition). The dashed red line in the figure on the center indicates what the specific heat at finite volume might be since $\mathrm{c}_{\theta_c^{-1}} = +\infty$. The right figure is a plot as a function of λ of the relative specific heat jump, i.e., the ratio $\Delta c / c_{\max}$ between the jump Δc at $\theta = \theta_c$ and the maximum value $c_{\max}$ of $\mathrm{c}_{\theta_c^{-1}}$ at the same point. The yellow colored area indicates that this ratio numerically computed is formally infinite due to a first order phase transition.*

Notice however that if experimental measurements of the specific heat comes from a *discrete* derivative of the mean energy per site ϵ_β, it is then clear that it corresponds to forget about the term $\mathfrak{C}_\beta$. In this case, i.e., assuming $\mathfrak{C}_\beta = 0$, we find again the well–known BCS–type behavior of the specific heat in presence of a second order phase transition, see figure 12. In addition, if $\mathfrak{C}_\beta = 0$, then for any μ, λ, h and $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$ (Corollary 3.5), we explicitly obtain via direct computations the well–known exponential decay of the specific heat at zero-temperature for s–wave superconductors:

$$\mathrm{c}_\beta = \frac{1}{4}\left(2\lambda\gamma + \gamma^2 - 4\lambda^2\right)\beta^2 e^{-\beta\gamma} + o\left(\beta^2 e^{-\beta\gamma}\right) \text{ as } \beta \to \infty. \tag{3.15}$$

(Note that this asymptotic could give access to γ and also λ, see discussions in Section 5.) However, if a first order phase transition appears, then the (infinite volume) mean energy per site ϵ_β is discontinuous at the critical temperature θ_c (cf. figure 11) and the specific heat $\mathrm{c}_{\theta_c^{-1}}$ is infinite. In figure 12 we give an illustration of the ratio $\Delta c/c_{\max}$ between the jump Δc at $\theta = \theta_c$ and the maximum value $c_{\max}$ of $\mathrm{c}_{\theta_c^{-1}}$. For most of standard superconductors[15] note that the measured values are between 0.6 and 0.7. Numerical computations suggest that this ratio $\Delta c/c_{\max}$ may always be bounded in our model by one as soon as a second order phase transition appears.

4. Phase diagram at fixed electron density per site

In any finite volume, the electron density per site is strictly increasing as a function of the chemical potential μ by strict convexity of the pressure. Therefore, for any fixed electron density $\rho \in (0, 2)$ there exists a unique $\mu_{N,\beta} = \mu_{N,\beta}(\rho, \lambda, \gamma, h)$ such that

$$\rho = \frac{1}{N}\sum_{x\in\Lambda_N} \omega_N\left(n_{x,\uparrow} + n_{x,\downarrow}\right), \tag{4.1}$$

where ω_N represents the (finite volume) grand–canonical Gibbs state (1.6) associated with H_N and taken at inverse temperature β and chemical potential $\mu = \mu_{N,\beta}$. The aim of this section is now to analyze the thermodynamic properties of the model for a fixed ρ instead of a fixed chemical potential μ. We start by investigating it away from any critical point.

4.1 Thermodynamics away from any critical point

In the thermodynamic limit and away from any critical point, the chemical potential $\mu_{N,\beta}$ converges to a solution $\mu_\beta = \mu_\beta(\rho, \lambda, \gamma, h)$ of the equation

$$\rho = \mathrm{d}_\beta\left(\mu, \lambda, \gamma, h\right), \tag{4.2}$$

see Theorem 3.8. For instance, if $\rho = 1$, the chemical potential μ_β is simply given by λ, i.e., $\mu_\beta(1, \lambda, \gamma, h) = \lambda$. At least away from any critical point, this chemical potential μ_β is always uniquely defined.

Indeed, outside the superconducting phase (see Section 3.1), the electron density d_β given by Theorem 3.8 is a strictly increasing continuous function of the chemical potential μ at fixed $\beta > 0$. In other words, for any fixed electron density $\rho \in (0, 2)$, the equation (4.2) has a unique solution μ_β, i.e., the chemical potential μ_β is the inverse of the electron density d_β taken as a function of $\mu \in \mathbb{R}$.

On the other hand, inside the superconducting phase, from (3.3) the chemical potential μ_β is also unique and equals

$$\mu_\beta = \frac{\gamma}{2}\left(\rho - 1\right) + \lambda, \tag{4.3}$$

see figures 5 and 10. In particular, μ_β does not depend on h or β as soon as $\mathrm{r}_\beta > 0$. The gap equation (2.5) then equals

$$\tanh\left(\beta\gamma\mathfrak{g}_r\right) = 2\mathfrak{g}_r\left(1 + \frac{e^{\lambda\beta}\cosh\left(\beta h\right)}{\cosh\left(\beta\gamma\mathfrak{g}_r\right)}\right), \text{ with } \mathfrak{g}_r := \frac{1}{2}\{(\rho-1)^2 + 4r\}^{1/2},$$

and

$$0 \leq \mathrm{r}_\beta \leq \max\left\{0, \rho\left(2-\rho\right)/4\right\},$$

[15] at least for the following elements: Hg, In, Nb, Pb, Sn, Ta, Tl, V.

for any fixed electron density $\rho \in (0,2)$.

Hence, the thermodynamic behavior of the strong coupling BCS–Hubbard model H_N is simply given for any $\rho \in (0,2)$, away from any critical point, by setting $\mu = \mu_\beta$ in Section 3. In particular, the superconducting phase can appear by tuning in each parameter: the BCS coupling constant γ (see (2.6)), the inverse temperature $\beta > 0$ (see Corollary 3.5), the coupling constant λ, the magnetic field h (see Section 3.3), the chemical potential μ or the electron density ρ (see Section 3.5). Therefore, to explain the phase diagram at fixed electron density, it is sufficient to give the behavior of the Cooper pair condensate density r_β as a function of $\rho \in (0,2)$. Everything can be easily performed via numerical methods, see figure 13. We restrict our rigorous analysis to the zero–temperature limit of r_β, which is a straightforward consequence of Corollary 3.5 and (4.3).

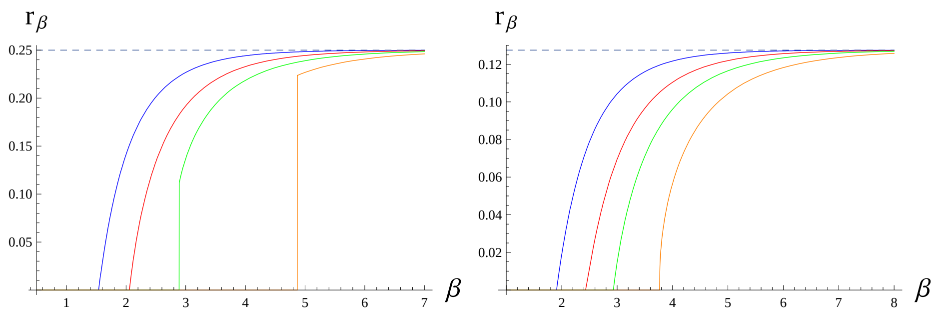

Figure 13: *Illustrations of the Cooper pair condensate density* r_β *as a function of the inverse temperature* β *for* $\gamma = 2.6$*,* $h = 0$*, and densities* $\rho = 1$*,* 1.7 *(respectively left and right figures), with* $\lambda = 0$ *(blue line),* 0.5 *(red line),* 0.75 *(green line), and* 1 *(orange line). The dashed line indicates the value of* r_∞*.*

Corollary 4.1 (Zero–temperature Cooper pair condensate density)
At zero–temperature, fixed electron density $\rho \in (0,2)$ *and* $\lambda, h \in \mathbb{R}$*, the Cooper pair condensate density* r_β *converges as* $\beta \to \infty$ *towards* $\mathrm{r}_\infty = \rho(2-\rho)/4$ *when* $\gamma > \max\{\tilde{\Gamma}_{\rho,\lambda+|h|}, 0\}$*. Here*

$$\tilde{\Gamma}_{x,y} := \frac{4y}{x\,(x-2)+2}\chi_{[0,\infty)}\,(y)$$

is a function defined for any $x, y \in \mathbb{R}$*.*

Remark 4.2 *The case* $0 < \gamma < \tilde{\Gamma}_{\rho,\lambda+|h|}$ *is more subtle than its analogous with a fixed chemical potential* μ*, because phase mixtures can take place. See Section 4.2.*

As explained above, as soon as $\gamma > \tilde{\Gamma}_{\rho,\lambda+|h|}$ we can extract from this corollary all the zero–temperature thermodynamics of the strong coupling BCS–Hubbard model by using Corollaries 3.5, 3.9, 3.11, and 3.13.

If $\lambda + |h| > 0$ and γ satisfy the inequalities

$$\gamma > \min_{\rho\in(0,2)} \left\{\tilde{\Gamma}_{\rho,\lambda+|h|}\right\} = \tilde{\Gamma}_{0,\lambda+|h|} = \tilde{\Gamma}_{2,\lambda+|h|} = 2\,(\lambda + |h|)$$

and

$$\gamma < \max_{\rho\in(0,2)} \left\{\tilde{\Gamma}_{\rho,\lambda+|h|}\right\} = \tilde{\Gamma}_{1,\lambda+|h|} = 4\,(\lambda + |h|)\,,$$

it is also clear that the superconductor–Mott insulator phase transition appears by tuning the electron density ρ in the same way as described in Section 3.5 for μ. See figures 10. In this case however, we recommend Section 4.2 for more details because of the subtlety mentioned in Remark 4.2. See figures 15-16 below.

From (4.3) combined with Corollary 4.1, note that the asymptotics (3.15) of the specific heat at zero-temperature is still valid at fixed electron density ρ as soon as $\gamma > \max\{\tilde{\Gamma}_{\rho,\lambda+|h|}, 0\}$. Meanwhile, from Corollary 4.1 the zero–temperature Cooper pair condensate density r_∞ does not depend on λ, γ, or h, as soon as $\gamma > \tilde{\Gamma}_{\rho,\lambda+|h|}$ is satisfied. Indeed, the chemical potential μ_β in the case where $\mathrm{r}_\beta > 0$ is renormalized, cf. (4.3).

In other words, at zero–temperature, the thermodynamic behavior of the strong coupling BCS–Hubbard model for $\gamma > \tilde{\Gamma}_{\rho,\lambda+|h|}$ is equal to the well–known behavior of the BCS theory in the strong coupling approximation ($\lambda = h = 0$). This phenomenon is also seen by using renormalization methods where it is believed that the Coulomb interaction simply modifies the mass of electrons by creating quasi–particles (which however do not exist in our model).

4.2 Coexistence of ferromagnetic and superconducting phases

Observe that the electron density d_β given by Theorem 3.8 can have discontinuities as a function of the chemical potential μ. This phenomenon appears at the superconductor–Mott insulator phase transition, see Section 3.5 and figure 10. Because of electron–hole symmetry (Section 3.2), without loss of generality we can restrict our study to the case where $\mathrm{d}_\beta \in [0,1]$, i.e., $\rho \in [0,1]$ and $\mu_\beta \leq \lambda$.

In this regime, the electron density d_β has, at most, one discontinuity point at the so-called *critical chemical potential* $\mu_\beta^{(c)} \leq \lambda$. In particular, there are two critical electron densities

$$\mathrm{d}_\beta^\pm := \mathrm{d}_\beta(\mu_\beta^{(c)} \pm 0, \lambda, \gamma, h) \quad \text{with } \mathrm{d}_\beta^+ > \mathrm{d}_\beta^-.$$

Similarly, we can also define two critical Cooper pair condensate densities $\mathrm{r}_\beta^\pm$, two critical magnetization densities[16] $\mathrm{m}_\beta^\pm$ and two critical Coulomb correlation density $\mathrm{w}_\beta^\pm$. Of course, since $\mathrm{r}_\beta^+ > \mathrm{r}_\beta^- = 0$, we are here on a critical point, i.e.,

$$(\beta, \mu_\beta^{(c)}, \lambda, \gamma, h) \in \partial\mathcal{S}$$

(see (2.7)), with $\beta, \gamma > 0$ and $\lambda, h \in \mathbb{R}$ such that this critical chemical potential $\mu_\beta^{(c)} = \mu_\beta^{(c)}(\lambda,\gamma,h)$ exists.

The thermodynamics of the model for $\rho \notin [\mathrm{d}_\beta^-, \mathrm{d}_\beta^+]$ is already explained in Section 4.1 because the solution r_β of (2.4) is unique at $\mu = \mu_\beta$. The chemical potential $\mu_{N,\beta}$ converges to $\mu_\beta = \mu_\beta^{(c)}$, if $\rho \in [\mathrm{d}_\beta^-, \mathrm{d}_\beta^+]$. In this case the variational problem (2.4) has exactly two maximizers $\mathrm{r}_\beta^\pm$. The thermodynamic behavior of the system in this regime is not, a priori, clear except from the obvious fact that

$$\lim_{N\to\infty} \frac{1}{N} \sum_{x\in\Lambda_N} \omega_N(n_{x,\uparrow} + n_{x,\downarrow}) = \rho$$

per definition. In particular, it cannot be deduced from the above results. We handle this situation within a much more general framework in Theorem 6.15. As a consequence of this study (see discussions after Theorem 6.15), all the extensive quantities can be obtained in the thermodynamic limit:

Theorem 4.3 (Densities in coexistent phases)
Take $\beta, \gamma > 0$ and real numbers λ, h in the domain of definition of the critical chemical potential $\mu_\beta^{(c)}$. For any $\rho \in [\mathrm{d}_\beta^-, \mathrm{d}_\beta^+]$, all densities are uniquely defined:
(i) The Cooper pair condensate density equals

$$\lim_{N\to\infty} \left\{ \frac{1}{N^2} \sum_{x,y\in\Lambda_N} \omega_N\left(a_{x,\uparrow}^* a_{x,\downarrow}^* a_{y,\downarrow} a_{y,\uparrow}\right) \right\} = \tau_\rho \mathrm{r}_\beta^+, \text{ with } \tau_\rho := \frac{\rho - \mathrm{d}_\beta^-}{\mathrm{d}_\beta^+ - \mathrm{d}_\beta^-} \in [0,1].$$

(ii) The magnetization density equals

$$\lim_{N\to\infty} \left\{ \frac{1}{N} \sum_{x\in\Lambda_N} \omega_N\left(n_{x,\uparrow} - n_{x,\downarrow}\right) \right\} = (1-\tau_\rho)\,\mathrm{m}_\beta^- + \tau_\rho \mathrm{m}_\beta^+.$$

(iii) The Coulomb correlation density equals

$$\lim_{N\to\infty} \left\{ \frac{1}{N} \sum_{x\in\Lambda_N} \omega_N\left(n_{x,\uparrow} n_{x,\downarrow}\right) \right\} = (1-\tau_\rho)\,\mathrm{w}_\beta^- + \tau_\rho \mathrm{w}_\beta^+.$$

[16] If $h = 0$, then $\mathrm{m}_\beta^\pm = 0$.

(iv) The mean energy per site equals

$$\lim_{N\to\infty}\left\{N^{-1}\omega_N\left(\mathrm{H}_N\right)\right\} = \left(1-\tau_\rho\right)\epsilon_\beta^- + \tau_\rho \epsilon_\beta^+,$$

with $\epsilon_\beta^\pm := -\mu_\beta^{(c)}\rho - h\mathrm{m}_\beta^\pm + 2\lambda \mathrm{w}_\beta^\pm - \gamma \mathrm{r}_\beta^\pm$.

As a consequence of this theorem, as soon as the magnetic field $h \neq 0$, there is a coexistence of ferromagnetic and superconducting phases at low temperatures for $\rho \in (\mathrm{d}_\beta^-, \mathrm{d}_\beta^+)$. In other words, the Meißner effect is not valid in this interval of electron densities. An illustration of this is given in figure 14. Such phenomenon was also observed in experiments and from our results, it should occur rather near half–filling (but *not exactly* at half–filling) and at strong repulsion $\lambda > 0$. Additionally, observe that this coexistence of thermodynamic phases can also appear at the critical magnetic field $\mathrm{h}_\beta^{(c)}$ (see Section 3.3).

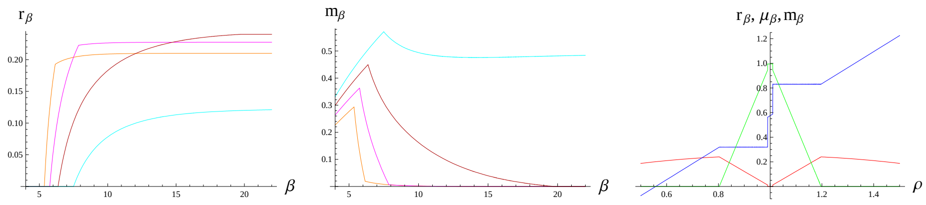

Figure 14: *In the two figures on the left, we give illustrations of the Cooper pair condensate density* r_β *and the magnetization density* m_β *as functions of the inverse temperature* β *for densities* $\rho = 0.6$ *(orange line),* 0.7 *(magenta line),* 0.8 *(red line),* 0.9 *(cyan line). In the figure on the right, we illustrate the coexistence of ferromagnetic and superconducting phases via graphs of* r_β*,* m_β *and the chemical potential* μ_β *as functions of* ρ *for* $\beta = 30$ *(low temperature regime). In all figures,* $\lambda = 0.575$*,* $\gamma = 2.6$*, and* $h = 0.1$*. (The small discontinuities around* $\rho = 1$ *in the right figure are numerical anomalies)*

Remark 4.4 *Coexistence of ferromagnetic and superconducting phases has already been rigorously investigated, see, e.g., [16, 17]. For instance, in [16] such phenomenon is shown to be impossible in the ground state of the Vonsovkii–Zener model applied to s–wave superconductors*[17]*, whereas at finite temperature, numerical computations [17] suggests the contrary. This last analysis [17] is however not performed in details.*

The second interesting physical aspect related to densities ρ between the critical densities d_β^- and d_β^+ is a smoothing effect of the extensive quantities (magnetization density, Cooper pair condensate density, etc.) as functions of the inverse temperature β. Indeed, since the critical chemical potential $\mu_\beta^{(c)}$ only exists when a first order phase transition occurs, one could expect that the extensive quantities are not continuous as functions of $\beta > 0$. In fact, for $\rho \in (\mathrm{d}_\beta^-, \mathrm{d}_\beta^+)$, there is a convex interpolation between quantities related to the solutions $\mathrm{r}_\beta^- = 0$ and $\mathrm{r}_\beta^+ > 0$ of (2.4), see Theorem 4.3. The continuity of the extensive quantities then follows, see figure 14. It does not imply however, that all densities become always continuous at fixed ρ as a function of the inverse temperature β. For instance, in figure 13, the green and orange graphs give two illustrations of a discontinuity of the order parameter r_β at fixed electron density $\rho = 1$ where $\mu_\beta = \lambda$. To understand this first order phase transition, other extensive quantity should be additionally fixed, see discussions in Section 5 and figure 17.

Following these last results, we give now in figure 15 other plots of the critical temperature $\theta_c = \theta_c(\rho, \lambda, \gamma, h)$, which is defined as usual such that $\mathrm{r}_\beta > 0$ if and only if $\beta > \theta_c^{-1}$. In this figure, observe that a positive λ, i.e., a one–site repulsion, can never increase the critical temperature if the electron density ρ is fixed instead of the chemical potential μ, compare with figure 2. We also show in figure 15 (right figure) that if the density of holes equals the density of electrons, i.e., $\rho = 1$, then we have a Mott insulator, whereas a small doping of electrons or holes implies either a superconducting phase (blue area) or a superconductor–Mott insulator (ferromagnetic) phase (yellow area) related to the superconductor–Mott insulator phase transition described in Section 3.5 and figure 10.

[17]It is a combination of the BCS interaction (1.3) with the Zener s–d exchange interaction.

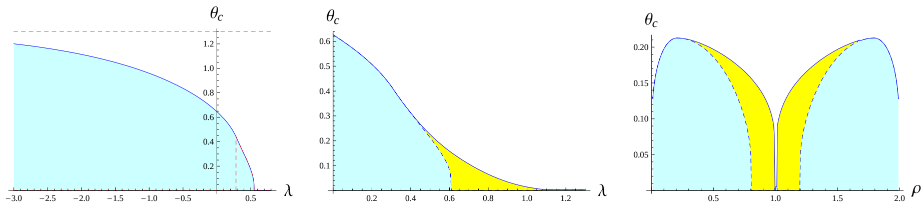

Figure 15: *Illustration, as a function of* λ *(the two figures on the left) or* ρ *(figure on the right), of the critical temperature* $\theta_c = \theta_c(\rho, \lambda, \gamma, h)$ *for* $\gamma = 2.6$, $h = 0.1$ *and with* $\rho = 1$ *(left figure),* $\rho = 0.7$ *(figure on the center) and* $\lambda = 0.575$ *(right figure). The blue and yellow area correspond respectively to the superconducting and ferromagnetic–superconducting phases, whereas the red dashed line indicates the domain of* λ *with a first order phase transition as a function of* β *or the temperature* $\theta := \beta^{-1}$ *(It only exists in the left figure). The dashed green line (left figure) is the asymptote when* $\lambda \to -\infty$. *In the right figure, observe that there is no phase transition for* $\rho = 1$.

To conclude, the figure 16 illustrates various thermodynamic features of the system at fixed ρ. First, as a function of $\beta > 0$, ϵ_β is continuously differentiable only for $\rho = 1$. In other words, there is no phase transition by opposition to the cases with $\rho = 0.7$, 0.9 or $\rho = 1.1$, 1.3. This is the Mott insulator phase transition illustrated in figure 10. As in figure 10, we also observe the electron–hole symmetry implying that $\rho = 0.7$ and $\rho = 1.3$, or $\rho = 0.9$ and $\rho = 1.1$, has same phase transitions at exactly the same critical points. As explained in Section 3.1, the mean energy per site ϵ_β for $\rho = 0.7$, 1.3, or $\rho = 0.9$, 1.1, differs by a constant, i.e., in absolute value by $|2\lambda - \mu_\beta|$. At high temperatures, i.e., when $\beta \to 0$, the function ϵ_β diverges to $\pm\infty$ if $\rho = 1 \mp \varepsilon$ with $\varepsilon \in (0, 1)$ whereas it stays finite at $\rho = 1$. Indeed, when $\beta \to 0$ the electron density d_β converges to 1 at fixed μ, λ, γ, h, see Theorem 3.8 and figure 5. If $\rho = 1 \mp \varepsilon$, it follows that the chemical potential μ_β diverges to $\mp\infty$ as $\beta \to 0$, implying that $\epsilon_\beta \to \pm\infty$. In other words, it is energetically unfavorable to fix an election density $\rho \neq 1$ at high temperatures. Finally, the specific heat c_β has only one jump in the case of one phase transition and two jumps when there are two phase transitions, namely when the superconductor–Mott insulator (ferromagnetic) phase and the purely superconducting phase appear.

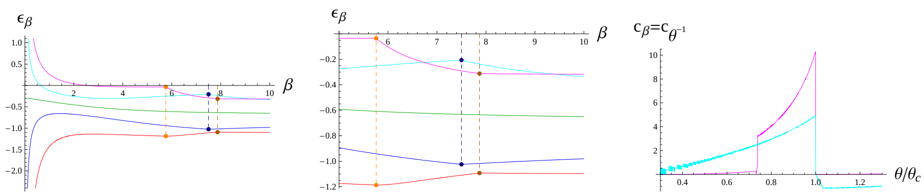

Figure 16: *In the two figures on the left, we give illustrations of the mean energy per site* ϵ_β *as a function of the inverse temperature* β *for densities* $\rho = 0.7$ *(magenta line),* 0.9 *(cyan line),* 1 *(green line),* 1.1 *(blue line) and* 1.3 *(red line). For* $\rho = 1$*, there is no phase transition and for* $\rho = 0.9$ *or* 1.1 *only a ferromagnetic-superconducting phase appears, whereas for* $\rho = 0.7$ *or* 1.3 *this last phase is followed for larger* β *by a superconducting phase. In the figure on the right, assuming* $\mathfrak{C}_\beta = 0$*, we give two plots of the specific heat* c_β *as a function of the ratio* θ/θ_c *between* $\theta := \beta^{-1}$ *and the critical temperature* θ_c *for densities* $\rho = 0.7$ *(magenta line) and* 0.9 *(cyan line). In all figures,* $\lambda = 0.575$*,* $\gamma = 2.6$*, and* $h = 0.1$.

5. Concluding remarks

1. First, it is important to note that two different physical behaviors can be extracted from the strong coupling BCS–Hubbard model H_N: a first one at fixed chemical potential μ and a second one at fixed electron density $\rho \in (0, 2)$. This does *not* mean that the canonical and grand–canonical ensembles are not equivalent for this model. But, the influence of the direct interaction with coupling constant λ drastically changes from the case at fixed μ to the other one at fixed ρ. For instance, via Corollary 4.1 (see also figure 15), any one–site repulsion between pairs of electrons is in any case unfavorable to the formation of Cooper pairs, as soon as the electron density ρ is fixed. This property is however wrong at fixed chemical potential μ, see figure 2. In other words, fixing the electron density ρ is *not* equivalent[18] to fixing the chemical potential μ in the model. Physically, a fixed electron density can be modified by doping the superconductor. Changing the chemical potential may be more difficult. One naive proposition would be to impose an electric potential on a superconductor which is coupled to an additional conductor serving as a reservoir of electrons or holes at fixed chemical potential.

2. A measurement of the asymptotics as $\beta \rightarrow \infty$ of the specific heat c_β (see (3.14) with $\mathfrak{C}_\beta = 0$) in a superconducting phase would determine, by using (3.15), first the parameter $\gamma > 0$ via the exponential decay and then the coupling constant λ. Next, the measurement of the critical magnetic field at very low temperature would allow to obtain by (3.5) the chemical potential μ and hence the electron density at zero–temperature. Since the inverse temperature β as well as the magnetic field h can directly be measured, all parameters of the strong coupling BCS–Hubbard model H_N (1.2) would be experimentally found. In particular, its thermodynamic behavior, explained in Sections 2–4, could finally be confronted to the real system. One could for instance check if the critical temperature θ_c given by H_N in appropriate dimension corresponds to the one measured in the real superconductor. Such studies would highlight the thermodynamic impact of the kinetic energy.

3. In Section 4, the electron density is fixed but one could have fixed each extensive quantity: the Cooper pair condensate density, the magnetization density, the Coulomb correlation density or the mean–energy per site. For instance, if the magnetization density $\mathrm{m} \in \mathbb{R}$ is fixed, by strict convexity of the pressure there is a unique magnetic field $h_{N,\beta} = h_{N,\beta}(\mu, \lambda, \gamma, m)$ such that

$$\mathrm{m} = \frac{1}{N} \sum_{x \in \Lambda_N} \omega_N \left(n_{x,\uparrow} - n_{x,\downarrow} \right).$$

In the thermodynamic limit, we then have $h_{N,\beta}$ converging to h_β solution of the equation $\mathrm{m}_\beta = \mathrm{m}$ at fixed $\beta, \gamma > 0$ and $\mu, \lambda \in \mathbb{R}$. By using Theorem 6.15, we would obtain the thermodynamics of the system for any $\beta, \gamma > 0$ and $\mu, \lambda, \mathrm{m} \in \mathbb{R}$. More generally, when one of the extensive quantities r_β, d_β, m_β, w_β, or ϵ_β is discontinuous at a critical point, then the thermodynamic limit of the local Gibbs states ω_N can be uniquely determined by fixing one of the corresponding extensive quantity between its critical values. The other extensive quantities are determined in this case by an obvious transcription of Theorem 4.3 for the considered discontinuous quantity at the critical point. Observe, however, that r_β, d_β, m_β, w_β, and ϵ_β should be related respectively to the parameters γ, μ, h, λ and β. For instance, the existence of a magnetic field $h_{N,\beta}$ solution of (4.1) at fixed $\rho \in (0, 2)$ is not clear at finite volume.

Figure 17 gives an example of an electron density always equal to 1 for $\mu = \lambda$ together with discontinuity of all other extensive quantities. In order to get well–defined quantities at the thermodynamic limit in this example for parameters allowing a first order phase transition, it is not sufficient to have the electron density fixed. At the critical point we could for instance fix the magnetization density $\mathrm{m} \in \mathbb{R}$ in the ferromagnetic case ($h = 0.1$) or in any case, the Coulomb correlation density $\mathrm{w} \geq 0$ which determines a coupling constant $\lambda_{N,\beta}$ converging to λ_β, see the right illustrations of figure 17 with the existence of a critical magnetic field and a critical coupling constant.

4. To conclude, as explained in the introduction, for a suitable space of states it is possible to define a free energy density functional $\mathfrak{F}$ (1.5) associated with the Hamiltonians H_N. The states minimizing this functional are equilibrium states and implies all the thermodynamics of the strong coupling BCS–Hubbard model discussed in Sections 3–4. Indeed, the weak*–limit ω_∞ of the local Gibbs state ω_N as $N \rightarrow \infty$ exists and belongs to our set of equilibrium states for any $\beta, \gamma > 0$ and $\mu, \lambda, h \in \mathbb{R}$, cf. Theorem 6.15. In Section 6.2, we prove in particular the following properties of equilibrium states:

(i) Any pure equilibrium state ω satisfies $\omega(a_{x,\downarrow} a_{x,\uparrow}) = \mathrm{r}_\beta^{1/2} e^{i\phi}$ for some $\phi \in [0, 2\pi)$. In particular, if $\mathrm{r}_\beta \neq 0$ they are not $U(1)$–gauge invariant and show *off diagonal long range order* [38] (ODLRO), cf. Theorems 6.10, 6.13 and Corollary 6.11.

[18] "Equivalent" is not taken here in the sense of the equivalence of ensembles.

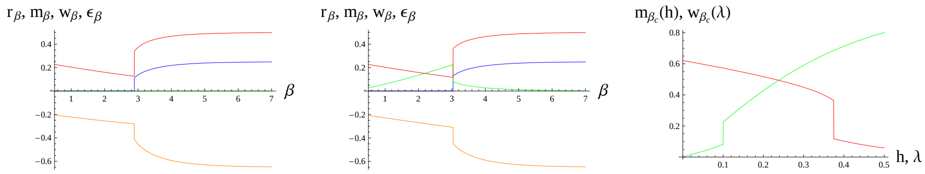

Figure 17: *In the two figures on the left, we give illustrations of the Cooper pair condensate density* r_β *(blue line), the magnetization density* m_β *(green line), the Coulomb correlation density* w_β *(red line), and the mean–energy per site* ϵ_β *(orange line) as functions of the inverse temperature* β *for* $h = 0$ *(figure on the left) and* $h = 0.1$ *(figure on the center) whereas* $\mu_\beta = \lambda = 0.375$*, i.e.,* $\rho = 1$*. In the figure on the right, we illustrate* m_{β_c} *(green line) and* w_{β_c} *(red line) respectively as functions of* h *with* $\mu = \lambda = 0.375$ *and* λ *with* $(\mu, h) = (0.375, 0.1)$ *at the critical inverse temperature* $\beta_c := \theta_c^{-1} \simeq 3.04$*.*

(ii) All densities are uniquely defined: the electron density of any equilibrium states ω is given by $\omega(n_{x,\uparrow} + n_{x,\downarrow}) = \mathrm{d}_\beta$, its magnetization density by $\omega(n_{x,\uparrow} - n_{x,\downarrow}) = \mathrm{m}_\beta$, and its Coulomb correlation density equals $\omega(n_{x,\uparrow}n_{x,\downarrow}) = \mathrm{w}_\beta$, cf. Theorem 6.14.

(iii) The Cooper fields $\Phi_x := a_{x,\downarrow}^* a_{x,\uparrow}^* + a_{x,\uparrow}a_{x,\downarrow}$ and $\Psi_x := i(a_{x,\downarrow}^* a_{x,\uparrow}^* - a_{x,\uparrow}a_{x,\downarrow})$ for pure states become classical in the limit $\gamma\beta \to \infty$, i.e., their fluctuations go to zero in this limit, cf. Theorem 6.16.

Any weak* limit point of equilibrium states with diverging inverse temperature is (by definition) a ground state. For $\gamma > 0$ and $\mu, \lambda, h \in \mathbb{R}$, most of ground states inherit the properties (i)-(iii) of equilibrium states. In particular, within the GNS–representation [32] of pure ground states, Cooper fields are exactly c–numbers, see Corollary 6.17. In this case, correlation functions can explicitly be computed at any order in Cooper fields. Furthermore, notice that even in the case $h = 0$ where the Hamiltonian H_N is spin invariant, there exist ground states breaking the spin $SU(2)$–symmetry. For more details including a precise formulation of these results, we recommend Section 6, in particular Section 6.2.

6. Mathematical foundations of the thermodynamic results

The aim of this section is to give all the detailed proofs of the thermodynamics of the strong coupling BCS–Hubbard model H_N (1.2). The central result of this section is the thermodynamic limit of the pressure, i.e., the proof of Theorem 2.1. The main ingredient in this analysis is the celebrated Størmer Theorem [1], which we adapt here for the CAR algebra (see Lemma 6.9). We orient our approach on the Petz–Raggio–Verbeure results in [19], but we would like to mention that the analysis of permutation invariant quantum systems in the thermodynamic limit (with Størmer's theorem as the background) is carried out for different classes of systems also by other authors. See, e.g., [33, 39]. Finally, we introduce in Section 6.2 a notion of equilibrium and ground states by a usual variational principle for the free energy density. The thermodynamics of the strong coupling BCS-Hubbard model described in Sections 3–4 is encoded in this notion and the thermodynamic limits of local Gibbs states used above for simplicity are special cases of equilibrium and ground states defined in Section 6.2. Before we proceed, we first define some basic mathematical objects needed in our analysis.

Let I be the set of finite subsets of $\mathbb{Z}^{d\geq 1}$. For any $\Lambda \in I$ we then define $\mathcal{U}_\Lambda$ as the C^*–algebra generated by $\{a_{x,\uparrow}, a_{x,\downarrow}\}_{x\in\Lambda}$ and the identity. Choosing some fixed bijective map $\kappa : \mathbb{N} \to \mathbb{Z}^d$, $\mathbb{N} := \{1, 2, \ldots\}$, $\mathcal{U}_N$ denotes the local C^*–algebra $\mathcal{U}_{\{\kappa(1),\ldots,\kappa(N)\}}$ at fixed $N \in \mathbb{N}$, whereas $\mathcal{U}$ is the full C^*–algebra, i.e., the closure of the union of all $\mathcal{U}_N$ for any integer $N \geq 1$. Note that

$$n_{\kappa(l),\uparrow} := a_{\kappa(l),\uparrow}^* a_{\kappa(l),\uparrow} \quad \text{and} \quad n_{\kappa(l),\downarrow} := a_{\kappa(l),\downarrow}^* a_{\kappa(l),\downarrow}$$

are the electron number operators on the site $\kappa(l)$, respectively with spin up $\uparrow$ and down $\downarrow$. To simplify the notation, as soon as a statement clearly concerns the one–site algebra $\mathcal{U}_1 = \mathcal{U}_{\{\kappa(1)\}}$, we replace $a_{\kappa(1),\uparrow}$, $a_{\kappa(1),\downarrow}$ and $n_{\kappa(1),\uparrow}$, $n_{\kappa(1),\downarrow}$ respectively by $a_\uparrow$, $a_\downarrow$ and $n_\uparrow$, $n_\downarrow$, whereas any state on $\mathcal{U}_1$ is denoted by ζ and not by ω, which is by definition a state on more than one site (on $\mathcal{U}_\Lambda$, $\mathcal{U}_N$ or $\mathcal{U}$). Important one–site Gibbs states in our analysis are the states ζ_c associated for any $c \in \mathbb{C}$ with the Hamiltonian $H_1(c)$ (2.1) and defined by

$$\zeta_c(A) := \frac{\text{Trace}\left(Ae^{\beta\left\{(\mu-h)n_\uparrow+(\mu+h)n_\downarrow+\gamma\left(ca_\downarrow^*a_\uparrow^*+\bar{c}a_\uparrow a_\downarrow\right)-2\lambda n_\uparrow n_\downarrow\right\}}\right)}{\text{Trace}\left(e^{\beta\left\{(\mu-h)n_\uparrow+(\mu+h)n_\downarrow+\gamma\left(ca_\downarrow^*a_\uparrow^*+\bar{c}a_\uparrow a_\downarrow\right)-2\lambda n_\uparrow n_\downarrow\right\}}\right)}, \tag{6.1}$$

for any $A \in \mathcal{U}_1$. Finally, note that our notation for the "Trace" does not include the Hilbert space where it is evaluated. Using the isomorphisms $\mathcal{U}_\Lambda \simeq B\left(\bigwedge \mathbb{C}^{\Lambda\times\{\uparrow,\downarrow\}}\right)$ of C^*–algebras, the corresponding Hilbert space is deduced from the local algebra where the operators involved in each statement are living.

Now, we are in position to start the proof of Theorem 2.1. It is followed by a rigorous analysis of the corresponding equilibrium and ground states.

6.1 Thermodynamic limit of the pressure: proof of Theorem 2.1

Since we have already shown the lower bound (2.2) in section 2, to finish the proof of Theorem 2.1 it remains to obtain

$$\limsup_{N\to\infty} \{\mathrm{p}_N(\beta,\mu,\lambda,\gamma,h)\} \leq \sup_{c\in\mathbb{C}} \left\{-\gamma|c|^2 + p(c)\right\}. \tag{6.2}$$

We split this proof into several lemmata. But first, we need some additional definitions.

We define the set of all S–invariant even states. Let S be the set of bijective maps from $\mathbb{N}$ to $\mathbb{N}$ which leaves invariant all but finitely many elements. It is a group w.r.t. the composition. The condition

$$\eta_s : a_{\kappa(l),\#} \mapsto a_{\kappa(s(l)),\#}, \quad s \in S,\ l \in \mathbb{N}, \tag{6.3}$$

defines a group homomorphism $\eta : S \to \mathrm{Aut}(\mathcal{U})$, $s \mapsto \eta_s$ uniquely. Here, $\#$ stands for a spin up $\uparrow$ or down $\downarrow$. Then, let

$$\begin{aligned} E_{\mathcal{U}}^{S,+} \quad := \quad & \big\{\omega \in E_{\mathcal{U}} :\ \omega \circ \eta_s = \omega \text{ for any } s \in S, \text{ and} \\ & \omega(a_{\kappa(l_1),\#}^* \cdots a_{\kappa(l_t),\#}^* a_{\kappa(m_1),\#} \cdots a_{\kappa(m_\tau),\#}) = 0 \text{ if } t+\tau \text{ is odd}\big\} \end{aligned}$$

be the set of all S–invariant even states, where $E_{\mathcal{U}}$ is the set of all states on $\mathcal{U}$. The set $E_{\mathcal{U}}^{S,+}$ is weak*–compact and convex. In particular, the set of extremal points of $E_{\mathcal{U}}^{S,+}$, denoted by $\mathcal{E}_{\mathcal{U}}^{S,+}$, is not empty.

Remark 6.1 *Any permutation invariant (p.i.) state on $\mathcal{U}$ is in fact automatically even, see, e.g., Example 5.2.21 of [25]. We explicitly write the evenness of states in the definition of $E_{\mathcal{U}}^{S,+}$ because this property is essential in our arguments below.*

Now, to fix the notation and for the reader convenience, we collect well–known results about the so–called relative entropy, cf. [25, 40]. Let $\omega^{(1)}$ and $\omega^{(2)}$ be two states on the local algebra $\mathcal{U}_\Lambda$, with $\omega^{(1)}$ being faithful. Define the relative entropy[19]

$$S(\omega^{(1)}|\omega^{(2)}) := \text{Trace}\left(D_{\omega^{(2)}} \ln D_{\omega^{(2)}}\right) - \text{Trace}\left(D_{\omega^{(2)}} \ln D_{\omega^{(1)}}\right),$$

where $D_{\omega^{(j)}}$ is the density matrix associated to the state $\omega^{(j)}$ with $j = 1, 2$. The relative entropy is super–additive: for any $\Lambda_1, \Lambda_2 \in I$, $\Lambda_1 \cap \Lambda_2 = \emptyset$, and for any even states $\omega^{(1)}, \omega^{(2)}, \omega^{(1,2)}$ respectively on $\mathcal{U}_{\Lambda_1}$, $\mathcal{U}_{\Lambda_2}$ and $\mathcal{U}_{\Lambda_1\cup\Lambda_2}$, $\omega^{(1)}$ and $\omega^{(2)}$ faithful, we have

$$S(\omega^{(1)} \otimes \omega^{(2)}\,|\,\omega^{(1,2)}) \geq S(\omega^{(1)}|\,\omega^{(1,2)}|_{\mathcal{U}_{\Lambda_1}}) + S(\omega^{(2)}\,|\,\omega^{(1,2)}|_{\mathcal{U}_{\Lambda_2}}). \tag{6.4}$$

For even states $\omega^{(1)}$ and $\omega^{(2)}$, respectively on $\mathcal{U}_{\Lambda_1}$ and $\mathcal{U}_{\Lambda_2}$ with $\Lambda_1 \cap \Lambda_2 = \emptyset$, the even state $\omega^{(1)} \otimes \omega^{(2)}$ is the unique extension of $\omega^{(1)}$ and $\omega^{(2)}$ on $\mathcal{U}_{\Lambda_1\cup\Lambda_2}$ satisfying for all $A \in \mathcal{U}_{\Lambda_1}$ and all $B \in \mathcal{U}_{\Lambda_2}$,

$$\omega^{(1)} \otimes \omega^{(2)}(AB) = \omega^{(1)}(A)\omega^{(2)}(B).$$

[19] As in [40] we use the Araki–Kosaki definition, which has opposite sign than the one given in [25].

The state $\omega^{(1)}\otimes\omega^{(2)}$ is called the *product* of $\omega^{(1)}$ and $\omega^{(2)}$. The product of even states is an associative operation. In particular, products of even states can be defined w.r.t. any countable set $\{\mathcal{U}_{\Lambda_n}\}_{n\in\mathbb{N}}$ of subalgebras of $\mathcal{U}$ with $\Lambda_m \cap \Lambda_n = \emptyset$ for $m \neq m$.

Observe that the relative entropy becomes additive w.r.t. product states: if $\omega^{(1,2)} = \hat{\omega}^{(1)} \otimes \hat{\omega}^{(2)}$, where $\hat{\omega}^{(1)}$ and $\hat{\omega}^{(2)}$ are two even states respectively on $\mathcal{U}_{\Lambda_1}$ and $\mathcal{U}_{\Lambda_2}$, then (6.4) is satisfied with equality. The relative entropy is also convex: for any states $\omega^{(1)}$, $\omega^{(2)}$, and $\omega^{(3)}$ on $\mathcal{U}_\Lambda$, $\omega^{(1)}$ faithful, and for any $\tau \in (0,1)$

$$S(\omega^{(1)}\,|\,\tau\omega^{(2)} + (1-\tau)\omega^{(3)}) \leq \tau S(\omega^{(1)}\,|\,\omega^{(2)}) + (1-\tau)S(\omega^{(1)}\,|\,\omega^{(3)}). \tag{6.5}$$

Meanwhile

$$\begin{aligned} S(\omega^{(1)}\,|\,\tau\omega^{(2)} + (1-\tau)\omega^{(3)}) \quad \geq \quad & \tau \log\tau + (1-\tau)\log(1-\tau) + \tau S(\omega^{(1)}\,|\,\omega^{(2)}) \\ & +(1-\tau)S(\omega^{(1)}\,|\,\omega^{(3)}), \end{aligned} \tag{6.6}$$

for any $\tau \in (0,1)$. Note that the relative entropy makes sense in a class of states on $\mathcal{U}$ much larger than that of even states on $\mathcal{U}_\Lambda$ (cf. [40]), but this is not needed here.

The condition

$$\sigma : a_{\kappa(l),\#} \mapsto a_{\kappa(l+1),\#}$$

uniquely defines a homomorphism σ on $\mathcal{U}$ called *right–shift* homomorphism. Any state ω on $\mathcal{U}$ such that $\omega = \omega\circ\sigma$ is called shift–invariant and we denote by $E_{\mathcal{U}}^{\sigma}$ the set of shift–invariant states on $\mathcal{U}$. An important class of shift–invariant states are product states ω_ζ obtained by "copying" some even state ζ of the one–site algebra $\mathcal{U}_1$ on all other sites, i.e.,

$$\omega_\zeta := \bigotimes_{k=0}^{\infty} \zeta\circ\sigma^k. \tag{6.7}$$

Such product states are important and used below as reference states. More generally, a state ω is L–periodic with $L \in \mathbb{N}$ if $\omega = \omega\circ\sigma^L$. For each $L\in\mathbb{N}$, the set of all L–periodic states from $E_{\mathcal{U}}$ is denoted by $E_{\mathcal{U}}^{\sigma^L}$.

Let ζ be any faithful even state on $\mathcal{U}_1$ and let ω be any L–periodic state on $\mathcal{U}$. It immediately follows from super–additivity (6.4) that for any $N, M \in \mathbb{N}$

$$S(\omega_\zeta|_{\mathcal{U}_{(M+N)L}}\,|\,\omega|_{\mathcal{U}_{(M+N)L}}) \geq S(\omega_\zeta|_{\mathcal{U}_{ML}}\,|\,\omega|_{\mathcal{U}_{ML}}) + S(\omega_\zeta|_{\mathcal{U}_{NL}}\,|\,\omega|_{\mathcal{U}_{NL}}).$$

In particular, the following limit exists

$$\tilde{S}(\zeta,\omega) := \lim_{N\to\infty} \frac{S(\omega_\zeta|_{\mathcal{U}_{NL}}\,|\,\omega|_{\mathcal{U}_{NL}})}{NL} = \sup_{N\in\mathbb{N}} \frac{S(\omega_\zeta|_{\mathcal{U}_{NL}}\,|\,\omega|_{\mathcal{U}_{NL}})}{NL} \tag{6.8}$$

and is the relative entropy density of ω w.r.t. the reference state ζ. This functional has the following important properties:

Lemma 6.2 (Properties of the relative entropy density)
At any fixed $L\in\mathbb{N}$, the relative entropy density functional $\omega\mapsto\tilde{S}(\zeta,\omega)$ is lower weak*–semicontinuous, i.e., for any faithful even state $\zeta\in E_{\mathcal{U}_1}$ and any $r\in\mathbb{R}$, the set

$$M_r := \left\{\omega \in E_{\mathcal{U}}^{\sigma^L} \;:\; \tilde{S}(\zeta,\omega) > r\right\}$$

is open w.r.t. the weak*–topology. It is also affine, i.e., for any faithful state $\zeta\in E_{\mathcal{U}_1}$ and states $\omega,\omega'\in E_{\mathcal{U}}^{\sigma^L}$

$$\tilde{S}(\zeta,\tau\omega + (1-\tau)\omega') = \tau\tilde{S}(\zeta,\omega) + (1-\tau)\tilde{S}(\zeta,\omega'),$$

with $\tau\in(0,1)$.

Proof: Without loss of generality, let $L=1$. From the second equality of (6.8),

$$M_r = \bigcup_{N\in\mathbb{N}} \{\omega\in E_{\mathcal{U}}^{\sigma} \;:\; S(\omega_\zeta|_{\mathcal{U}_N}\,|\,\omega|_{\mathcal{U}_N}) > rN\}\,.$$

As the maps $\omega \mapsto S(\omega_\zeta|_{\mathcal{U}_N} \,|\, \omega|_{\mathcal{U}_N})$ are weak*–continuous for each N, it follows that M_r is the union of open sets, which implies the lower weak*–semicontinuity of the relative entropy density functional. Moreover from (6.5) and (6.6) we directly obtain that $\tilde{S}(\zeta,\omega)$ is affine. □

Notice that any p.i. state is automatically shift–invariant. Thus, the mean relative entropy density is a well–defined functional on $E_{\mathcal{U}}^{S,+}$. Now, we need to define on $E_{\mathcal{U}}^{S,+}$ the functional $\Delta(\omega)$ relating to the mean BCS interaction energy per site:

Lemma 6.3 (BCS energy per site for p.i. states)
For any $\omega \in E_{\mathcal{U}}^{S,+}$, the mean BCS interaction energy per site in the thermodynamic limit

$$\begin{aligned}\Delta(\omega) &:= \lim_{N\to\infty} \frac{\gamma}{N^2} \sum_{l,m=1}^{N} \omega\left(a_{\kappa(l),\uparrow}^* a_{\kappa(l),\downarrow}^* a_{\kappa(m),\downarrow} a_{\kappa(m),\uparrow}\right) \\ &= \gamma\omega\left(a_{\kappa(1),\uparrow}^* a_{\kappa(1),\downarrow}^* a_{\kappa(2),\downarrow} a_{\kappa(2),\uparrow}\right)\end{aligned}$$

is well–defined and the affine map $\Delta : E_{\mathcal{U}}^{S,+} \to \mathbb{C}$, $\omega \mapsto \Delta(\omega)$ is weak–continuous.*

Proof: First,

$$\begin{aligned}\sum_{l,m=1}^{N} \omega\left(a_{\kappa(l),\uparrow}^* a_{\kappa(l),\downarrow}^* a_{\kappa(m),\downarrow} a_{\kappa(m),\uparrow}\right) &= \sum_{l=1}^{N} \omega\left(a_{\kappa(l),\uparrow}^* a_{\kappa(l),\downarrow}^* a_{\kappa(l),\downarrow} a_{\kappa(l),\uparrow}\right) \\ &\quad + \sum_{\substack{l,m=1 \\ l\neq m}}^{N} \omega\left(a_{\kappa(l),\uparrow}^* a_{\kappa(l),\downarrow}^* a_{\kappa(m),\downarrow} a_{\kappa(m),\uparrow}\right).\end{aligned} \tag{6.9}$$

Since $\omega \in E_{\mathcal{U}}^{S,+}$, for any $l \neq m$ observe that

$$\omega\left(a_{\kappa(l),\uparrow}^* a_{\kappa(l),\downarrow}^* a_{\kappa(m),\downarrow} a_{\kappa(m),\uparrow}\right) = \omega\left(a_{\kappa(1),\uparrow}^* a_{\kappa(1),\downarrow}^* a_{\kappa(2),\downarrow} a_{\kappa(2),\uparrow}\right), \tag{6.10}$$

whereas

$$\omega\left(a_{\kappa(l),\uparrow}^* a_{\kappa(l),\downarrow}^* a_{\kappa(l),\downarrow} a_{\kappa(l),\uparrow}\right) = \omega\left(a_{\kappa(1),\uparrow}^* a_{\kappa(1),\downarrow}^* a_{\kappa(1),\downarrow} a_{\kappa(1),\uparrow}\right). \tag{6.11}$$

Therefore, by combining (6.9) with (6.10) and (6.11), the lemma follows. □

Now, we define by

$$\omega^H(A) := \frac{\mathrm{Trace}\left(A\, e^{-\beta H}\right)}{\mathrm{Trace}\left(e^{-\beta H}\right)}, \quad A \in \mathcal{U}_\Lambda, \tag{6.12}$$

the Gibbs state associated with any self–adjoint element H of $\mathcal{U}_\Lambda$ at inverse temperature $\beta > 0$. This definition is of course in accordance with the Gibbs state ω_N (1.6) associated with the Hamiltonian[20] H_N (1.2) since $\omega_N = \omega^{\mathrm{H}_N}$ for any $N \in \mathbb{N}$. Note however, that the state ω_N is seen either as defined on the local algebra $\mathcal{U}_N$ or as defined on the whole algebra $\mathcal{U}$ by periodically extending it (with period N).

Next we give an important property of Gibbs states (6.12):

Lemma 6.4 (Passivity of Gibbs states)
Let H_0, H_1 be self–adjoint elements from $\mathcal{U}_\Lambda$ and define for any state ω on $\mathcal{U}_\Lambda$

$$F_\Lambda(\omega) := -\omega(H_1) - \beta^{-1} S(\omega^{H_0}|\omega) + P^{H_0},$$

where $P^H := \beta^{-1} \ln \mathrm{Trace}\left(e^{-\beta H}\right)$ for any self–adjoint $H \in \mathcal{U}_\Lambda$. Then $P^{H_1+H_0} \geq F_\Lambda(\omega)$ for any state ω on $\mathcal{U}_\Lambda$ with equality if $\omega = \omega^{H_0+H_1}$. Note that $-F_\Lambda(\omega)$ is the free energy associated with the state ω.

[20]with the appropriate numbering of sites defined by the bijective map κ.

Proof: For any self–adjoint $H \in \mathcal{U}_\Lambda$ and any state ω on $\mathcal{U}_\Lambda$ observe that

$$\mathrm{Trace}\,(D_\omega \ln D_{\omega^H}) = \mathrm{Trace}\left(D_\omega \ln \left(\exp\left(-\beta P^H - \beta H\right)\right)\right) = -\beta\omega(H) - \beta P^H, \tag{6.13}$$

which implies that

$$\begin{aligned} P^{H_1+H_0} \quad &= \quad -\beta^{-1}\left(\mathrm{Trace}\,(D_{\omega^{H_0+H_1}} \ln D_{\omega^{H_0+H_1}}) - \mathrm{Trace}\,(D_{\omega^{H_0+H_1}} \ln D_{\omega^{H_0}})\right) \\ &\quad -\omega^{H_0+H_1}(H_1) + P^{H_0}, \end{aligned} \tag{6.14}$$

i.e., $P^{H_1+H_0} = F_\Lambda(\omega^{H_0+H_1})$. Without loss of generality take any faithful state ω on $\mathcal{U}_\Lambda$. In this case, there are positive numbers λ_j with $\sum_j \lambda_j = 1$ and vectors $\langle j|$ from the Hilbert space $\bigwedge \mathcal{H}_\Lambda$ such that $\omega(\cdot) = \sum_j \lambda_j \langle j| \cdot |j\rangle$. In particular, from (6.13) we have

$$-\beta\omega(H_1) - S(\omega^{H_0}|\omega) + \beta P^{H_0} = \sum_j \lambda_j \left(-\ln\lambda_j - \beta\, \langle j|\, H_0 + H_1\, |j\rangle\right).$$

Consequently, by convexity of the exponential function combined with Jensen inequality we obtain that

$$\begin{aligned} &\exp\Big(-\beta\omega(H_1) - S(\omega^{H_0}|\omega) + \beta P^{H_0}\Big) \\ \leq\ &\sum_j \lambda_j \exp\left(-\ln\lambda_j - \beta\,\langle j|\, H_0 + H_1\, |j\rangle\right) \\ \leq\ &\mathrm{Trace}\,\left(\exp\left(-\beta(H_0+H_1)\right)\right) = \exp\left(\beta P^{H_1+H_0}\right). \end{aligned}$$

Note that the last inequality uses the so–called Peierls–Bogoliubov inequality which is again a consequence of Jensen inequality. □

This proof is standard (see, e.g., [25]). It is only given in detail here, because we also need later equations (6.13) and (6.14).

Observe that Lemma 6.4 applied to $\omega = \omega^{H_0}$ gives the Bogoliubov (convexity) inequality [29]. We can also deduce from this lemma that the pressure $\mathrm{p}_N\,(\beta,\mu,\lambda,\gamma,h)$ (1.4) associated with H_N equals

$$\begin{aligned} \mathrm{p}_N\,(\beta,\mu,\lambda,\gamma,h) \quad &= \quad \frac{\gamma}{N^2}\sum_{l,m=1}^{N} \omega_N\left(a_{\kappa(l),\uparrow}^* a_{\kappa(l),\downarrow}^* a_{\kappa(m),\downarrow} a_{\kappa(m),\uparrow}\right) \\ &\quad -\frac{1}{\beta N} S\left(\omega_{\zeta_0}|_{\mathcal{U}_N}|\omega_N\right) + \mathrm{p}_N\,(\beta,\mu,\lambda,0,h), \end{aligned} \tag{6.15}$$

for any $\beta,\gamma > 0$ and real numbers μ,λ,h. Recall that ω_{ζ_0} is the shift–invariant state obtained by "copying" the state ζ_0 (6.1) of the one–site algebra $\mathcal{U}_1$, see (6.7).

Lemma 6.5 (From S to the relative entropy density $\tilde{S}$ at finite N)
Let $\tilde{\omega}_N$ be the shift–invariant state defined by

$$\tilde{\omega}_N := \frac{1}{N}\left(\omega_N + \omega_N\circ\sigma + \cdots + \omega_N\circ\sigma^{N-1}\right),$$

where σ is the right–shift homomorphism. Then $S\left(\omega_{\zeta_0}|_{\mathcal{U}_N}|\omega_N\right) = N\tilde{S}\left(\zeta_0,\tilde{\omega}_N\right)$, cf. (6.8).

Proof: By Lemma 6.2 combined with (6.8), the relative entropy density $\tilde{S}\left(\zeta_0,\tilde{\omega}_N\right)$ equals

$$\tilde{S}\left(\zeta_0,\tilde{\omega}_N\right) = \lim_{M\to\infty}\left\{\frac{1}{MN}\sum_{k=0}^{N-1}\frac{1}{N} S\left(\omega_{\zeta_0}|_{\mathcal{U}_{MN}}\,|\,\omega_N\circ\sigma^k|_{\mathcal{U}_{MN}}\right)\right\}, \tag{6.16}$$

for any fixed $N \in \mathbb{N}$. By using now the additivity of the relative entropy for product states observe that

$$\begin{aligned} S\left(\omega_{\zeta_0}|_{\mathcal{U}_{MN}}\,|\,\omega_N\circ\sigma^k|_{\mathcal{U}_{MN}}\right) \quad &= \quad (M-1) S\left(\omega_{\zeta_0}|_{\mathcal{U}_N}\,|\,\omega_N|_{\mathcal{U}_N}\right) + S\left(\omega_{\zeta_0}|_{\mathcal{U}_k}\,|\,\omega_N|_{\mathcal{U}_k}\right) \\ &\quad + S\left(\omega_{\zeta_0}|_{\mathcal{U}_{N-k}}\,|\,\omega_N|_{\mathcal{U}_{N-k}}\right), \end{aligned} \tag{6.17}$$

for any $k \in \{0, \cdots, N-1\}$, with $S\left(\omega_{\zeta_0}|_{\mathcal{U}_0} \,|\, \omega_N|_{\mathcal{U}_0}\right) := 0$ by definition. Therefore the equality $S\left(\omega_{\zeta_0}|_{\mathcal{U}_N}|\omega_N\right) = N\tilde{S}\left(\zeta_0, \tilde{\omega}_N\right)$ directly follows from (6.16) combined with (6.17). □

We are now in position to give a first general upper bound for the pressure $\mathrm{p}_N\left(\beta, \mu, \lambda, \gamma, h\right)$ by using the equality (6.15) together with Lemmata 6.3 and 6.5.

Lemma 6.6 (General upper bound of the pressure p_N)
For any $\beta, \gamma > 0$ and $\mu, \lambda, h \in \mathbb{R}$, one gets that

$$\limsup_{N\rightarrow\infty} \left\{\mathrm{p}_N\left(\beta, \mu, \lambda, \gamma, h\right)\right\} \leq \mathrm{p}\left(\beta, \mu, \lambda, 0, h\right) + \sup_{\omega\in\mathcal{E}_{\mathcal{U}}^{S,+}} \left\{\Delta\left(\omega\right) - \beta^{-1}\tilde{S}\left(\zeta_0, \omega\right)\right\},$$

where we recall that $\mathcal{E}_{\mathcal{U}}^{S,+}$ is the non empty set of extremal points of $E_{\mathcal{U}}^{S,+}$.

Proof: By (6.15) combined with Lemma 6.5 one gets

$$\begin{aligned} \mathrm{p}_N\left(\beta, \mu, \lambda, \gamma, h\right) &= \frac{\gamma}{N^2}\sum_{l,m=1}^{N} \omega_N\left(a_{\kappa(l),\uparrow}^* a_{\kappa(l),\downarrow}^* a_{\kappa(m),\downarrow} a_{\kappa(m),\uparrow}\right) \\ &\quad -\beta^{-1}\tilde{S}\left(\zeta_0, \tilde{\omega}_N\right) + \mathrm{p}_N\left(\beta, \mu, \lambda, 0, h\right). \end{aligned} \tag{6.18}$$

The last term of this equality is independent of $N \in \mathbb{N}$ since

$$\mathrm{p}_N\left(\beta, \mu, \lambda, 0, h\right) = \frac{1}{\beta}\ln\mathrm{Trace}\left(e^{\beta[(\mu-h)n_\uparrow + (\mu+h)n_\downarrow - 2\lambda n_\uparrow n_\downarrow]}\right) =: \mathrm{p}\left(\beta, \mu, \lambda, 0, h\right), \tag{6.19}$$

cf. (2.3).

However, the other terms require the knowledge of the states ω_N and $\tilde{\omega}_N$ in the limit $N \rightarrow \infty$. Actually, because the unit ball in $\mathcal{U}$ is a metric space w.r.t. the weak*–topology, the sequence $\{\tilde{\omega}_N\}$ converges in the weak*–topology along a subsequence towards ω_∞. Meanwhile, it is easy to see that for all $A \in \mathcal{U}_\Lambda$, $\Lambda \in I$,

$$\lim_{N\rightarrow\infty} \left\{\omega_N\left(A\right) - \tilde{\omega}_N\left(A\right)\right\} = 0.$$

Thus, the sequences of states ω_N and $\tilde{\omega}_N$ have the same limit points. Since ω_N is even and permutation invariant w.r.t. the N first sites, the state ω_∞ belongs to $E_{\mathcal{U}}^{S,+}$. We now estimate the first term (6.18) as in Lemma 6.3 to get

$$\begin{aligned} \limsup_{N\rightarrow\infty}\left\{\mathrm{p}_N\left(\beta, \mu, \lambda, \gamma, h\right)\right\} &\leq \mathrm{p}\left(\beta, \mu, \lambda, 0, h\right) + \gamma\omega_\infty\left(a_{\kappa(1),\uparrow}^* a_{\kappa(1),\downarrow}^* a_{\kappa(2),\uparrow} a_{\kappa(2),\downarrow}\right) \\ &\quad + \beta^{-1}\limsup_{N\rightarrow\infty}\left\{-\tilde{S}\left(\zeta_0, \tilde{\omega}_N\right)\right\}. \end{aligned} \tag{6.20}$$

From Lemma 6.2 the relative entropy density is lower semicontinuous in the weak*–topology, which implies that

$$\limsup_{N\rightarrow\infty}\left\{-\tilde{S}\left(\zeta_0, \tilde{\omega}_N\right)\right\} \leq -\tilde{S}\left(\zeta_0, \omega_\infty\right).$$

By combining this last inequality with (6.20) we then find that

$$\limsup_{N\rightarrow\infty}\left\{\mathrm{p}_N\left(\beta, \mu, \lambda, \gamma, h\right)\right\} \leq \mathrm{p}\left(\beta, \mu, \lambda, 0, h\right) + \Delta\left(\omega_\infty\right) - \beta^{-1}\tilde{S}\left(\zeta_0, \omega_\infty\right), \tag{6.21}$$

with $\omega_\infty \in E_{\mathcal{U}}^{S,+}$.

Now, from Lemma 6.3 the functional $\omega \mapsto \Delta(\omega)$ is affine and weak*–continuous, whereas by Lemma 6.2 the map $\omega \mapsto \tilde{S}(\zeta_0, \omega)$ is affine and lower weak*–semicontinuous. The free energy functional $\omega \mapsto \Delta(\omega) - \beta^{-1}\tilde{S}(\zeta_0, \omega)$ is, in particular, convex and upper weak*–semicontinuous. Meanwhile recall that $E_{\mathcal{U}}^{S,+}$ is a weak*–compact and convex set. Therefore, from the Bauer maximum principle [32, Lemma 4.1.12] it follows that

$$\sup_{\omega\in E_{\mathcal{U}}^{S,+}}\left\{\Delta\left(\omega\right) - \beta^{-1}\tilde{S}\left(\zeta_0, \omega\right)\right\} = \sup_{\omega\in\mathcal{E}_{\mathcal{U}}^{S,+}}\left\{\Delta\left(\omega\right) - \beta^{-1}\tilde{S}\left(\zeta_0, \omega\right)\right\}. \tag{6.22}$$

Together with (6.21), this last inequality implies the upper bound stated in the lemma. □

Since even states on $\mathcal{U}$ are entirely determined by their action on even elements from $\mathcal{U}$, observe that we can identify the set of even p.i. states of $\mathcal{U}$ with the set of p.i. states on the even sub–algebra $\mathcal{U}^+$. We want to show next that the set of extremal points $\mathcal{E}_{\mathcal{U}}^{S,+}$ belongs to the set of strongly clustering states on the even sub–algebra $\mathcal{U}^+$ of $\mathcal{U}$. By strongly clustering states ω w.r.t. $\mathcal{U}^+$, we mean that for any B in $\mathcal{U}^+$, there exists a net $\{B_j\} \subseteq \mathrm{Co}\{\eta_s(B) : s \in S\}$ such that for any $A \in \mathcal{U}^+$,

$$\lim_j |\omega\left(A\,\eta_s\left(B_j\right)\right) - \omega\left(A\right)\omega\left(B\right)| = 0$$

uniformly in $s \in S$. Here, $\mathrm{Co}\, M$ denotes the convex hull of the set M.

Lemma 6.7 (Characterization of the set of extremal states of $E_{\mathcal{U}}^{S,+}$)
Any extremal state $\omega \in \mathcal{E}_{\mathcal{U}}^{S,+}$ is strongly clustering w.r.t. the even sub–algebra $\mathcal{U}^+$ and conversely.

Proof: We use some standard facts about extremal decompositions of states which can be found in [32, Theorems 4.3.17 and 4.3.22]. To satisfy the requirements of these theorems, we need to prove that the C^*–algebra $\mathcal{U}^+$ of even elements of $\mathcal{U}$ is asymptotically abelian w.r.t. the action of the group S. This is proven as follows. For each $l \in \mathbb{N}$ define the map $\pi^{(l)} : \mathbb{N} \to \mathbb{N}$ by

$$\pi^{(l)}(k) := \begin{cases} k + 2^{l-1} & , \quad \text{if } 1 \leq k \leq 2^{l-1}. \\ k - 2^{l-1} & , \quad \text{if } 2^{l-1}+1 \leq k \leq 2^l. \\ k & , \quad \text{if } k > 2^l. \end{cases} \tag{6.23}$$

In other words, the map $\pi^{(l)}$ exchanges the block $\{1, \cdots, 2^{l-1}\}$ with $\{2^{l-1}+1, \cdots, 2^l\}$, and leaves the rest invariant. For any $A, B \in \mathcal{U}_\Lambda \cap \mathcal{U}^+$ with $\Lambda \in I$, it is then not difficult to see that

$$\lim_{l\to\infty} [A, \eta_{\pi^{(l)}}\left(B\right)] = 0$$

in the norm sense. Recall that the map $\eta_{\pi^{(l)}}$ is defined via (6.3). By density of local elements of $\mathcal{U}^+$ the limit above equals zero for all $A, B \in \mathcal{U}^+$. Therefore, by using now [32, Theorems 4.3.17 and 4.3.22] all states $\omega \in \mathcal{E}_{\mathcal{U}}^{S,+}$ are then strongly clustering w.r.t. $\mathcal{U}^+$ and conversely. □

We show next that p.i. states, which are strongly clustering w.r.t. the even sub–algebra $\mathcal{U}^+$, have clustering properties w.r.t. the whole algebra $\mathcal{U}$.

Lemma 6.8 (Extension of the strongly clustering property)
Let $\omega \in E_{\mathcal{U}}^{S,+}$ be any strongly clustering state w.r.t. $\mathcal{U}^+$. Then, for any $A, B \in \mathcal{U}$ and $\varepsilon > 0$, there are $B_\varepsilon \in \mathrm{Co}\{\eta_s(B) \ : \ s \in S\}$ and l_ε such that for any $l \geq l_\varepsilon$,

$$|\omega(A\eta_{\pi^{(l)}}(B_\varepsilon)) - \omega(A)\omega(B)| < \varepsilon.$$

Proof: By density of local elements it suffices to prove the lemma for any $A, B \in \mathcal{U}_N$ and $N \in \mathbb{N}$. The operators A and B can always be written as sums $A = A^+ + A^-$ and $B = B^+ + B^-$, where A^+ and B^+ are in the even sub–algebra $\mathcal{U}^+$ whereas A^- and B^- are odd elements, i.e., they are sums of monomials of odd degree in annihilation and creation operators. Since ω is assumed to be strongly clustering w.r.t. $\mathcal{U}^+$, for any $\varepsilon > 0$ there are positive numbers $\lambda_1, \ldots, \lambda_k$ with $\lambda_1 + \cdots + \lambda_k = 1$, and maps $s_1, \ldots, s_k \in S$ such that for any $l \in \mathbb{N}$,

$$\left|\omega\Big(A^+\,\eta_{\pi^{(l)}}\Big(\sum_{j=1}^{k} \lambda_k \eta_{s_j}(B^+)\Big)\Big) - \omega(A^+)\omega(B^+)\right| < \varepsilon. \tag{6.24}$$

By parity and linearity of ω observe that $\omega(A^+)\omega(B^+) = \omega(A)\omega(B)$, whereas

$$\omega(A\eta_{\pi^{(l)}}(B_\varepsilon)) = \omega\Big(A^+\,\eta_{\pi^{(l)}}\Big(\sum_{j=1}^{k} \lambda_k \eta_{s_j}(B^+)\Big)\Big) \tag{6.25}$$

for large enough l with the operator $B_\varepsilon \in \mathrm{Co}\{\eta_s(B) \ : \ s \in S\}$ defined by

$$B_\varepsilon := \sum_{j=1}^{k} \lambda_k \eta_{s_j}(B). \tag{6.26}$$

The equality (6.25) follows from parity and the statement

$$\omega(A\eta_{\pi^{(l)}}(\tilde{B}^-)) = 0$$

for any $\omega \in E_{\mathcal{U}}^{S,+}$, $A, \tilde{B}^- \in \mathcal{U}_N$, $\tilde{B}^-$ odd, and sufficiently large l. This can be seen as follows. Since any element of $\mathcal{U}_N$ with defined parity can be written as a linear combination of two self–adjoint elements with same parity, we assume without loss of generality that $(\tilde{B}^-)^* = \tilde{B}^-$. Choose $l' \in \mathbb{N}$ large enough such that the support of $\tilde{B}_l^- := \pi^{(l)}(\tilde{B}^-)$ does not intersect $\{\kappa(1), ..., \kappa(N)\}$ for all $l \geq l'$. The map $\pi^{(l)} : \mathbb{N} \to \mathbb{N}$ is defined by (6.23). Define $\tilde{B}_{l,m}^- := \sigma^{m2^{l+1}}(\tilde{B}_l^-)$, $m \in \mathbb{N}_0 := \{0, 1, 2, \ldots\}$, where σ is the right–shift homomorphism. For any $J \in \mathbb{N}$

$$\omega\Big(\sum_{m=0}^{J} A\tilde{B}_{l,m}^-\Big) = (J+1)\omega(A\tilde{B}_{l,0}^-)$$

by symmetry of ω. Use now the Cauchy–Schwarz inequality for states to get

$$(J+1)|\omega(A\tilde{B}_{l,0}^-)| \leq \sqrt{\omega(A^*A)}\sqrt{\sum_{m,m'=0}^{J} \omega(\tilde{B}_{l,m}^- \tilde{B}_{l,m'}^-)}.$$

Since per construction, $\tilde{B}_{l,m}^-$ and $\tilde{B}_{l,m'}^-$ anti–commute if $m \neq m'$,

$$\sum_{m,m'=0}^{J} \omega(B_{l,m}B_{l,m'}) = \sum_{m=0}^{J} \omega(B_{l,m}B_{l,m}).$$

By symmetry of ω, the right–hand side of the equation above equals $(J+1)\omega((\tilde{B}_{l,0}^-)^2)$. Hence, we conclude that

$$|\omega(A\tilde{B}_{l,0}^-)| \leq (J+1)^{-1/2}\sqrt{\omega(|A|^2)\omega((\tilde{B}_{l,0}^-)^2)},$$

for any $J \in \mathbb{N}$, i.e., $\omega(A\tilde{B}_{l,0}^-) = 0$ for all $l \geq l'$.

Therefore, the lemma follows from (6.24)–(6.25) with $B_\varepsilon \in \mathrm{Co}\{\eta_s(B) \ : \ s \in S\}$ defined by (6.26) for any $\varepsilon > 0$. ☐

We now identify the set of clustering states on $\mathcal{U}$ with the set of product states by the following lemma, which is a non–commutative version of de Finetti Theorem of probability theory [28]. Størmer [1] was the first to show the corresponding result for infinite tensor products of C^*–algebras.

Lemma 6.9 (Strongly clustering p.i. states are product states)
Any p.i. and strongly clustering (in the sense of Lemma 6.8) state ω is a product state (6.7) with the one–site state $\zeta = \zeta_\omega := \omega|_{\mathcal{U}_1}$ being the restriction of ω on the local (one–site) algebra $\mathcal{U}_1$.

Proof: Let $l_1, \ldots, l_k \in \mathbb{N}$ with $l_i \neq l_j$ whenever $i \neq j$, and for any $j \in \{1, \ldots, k\}$ take $A_j \in \mathcal{U}_1$. To prove the lemma we need to show that

$$\omega(\sigma^{l_1}(A_1) \ldots \sigma^{l_k}(A_k)) = \zeta_\omega(A_1) \ldots \zeta_\omega(A_k). \tag{6.27}$$

The proof of this last equality for any $k \geq 1$ is performed by induction. First, for $k = 1$ the equality (6.27) immediately follows by symmetry of the state ω. Now, assume the equality (6.27) verified at fixed $k \geq 1$. The state ω is strongly clustering in the sense of Lemma 6.8. Therefore for each $\varepsilon > 0$ there are $q \in \mathbb{N}$, positive numbers $\lambda_1, \ldots, \lambda_q$ with $\lambda_1 + \cdots + \lambda_q = 1$, and maps $s_1, \ldots, s_q \in S$ such that

$$\begin{aligned}&\Big|\textstyle\sum_{j=1}^{q} \lambda_j \omega\left(\sigma^{l_1}(A_1) \ldots \sigma^{l_k}(A_k)\, \eta_{\pi^{(l)} \circ s_j}\left(\sigma^{l_{k+1}}(A_{k+1})\right)\right)\\ &-\omega\left(\sigma^{l_1}(A_1) \ldots \sigma^{l_k}(A_k)\right)\omega\left(\sigma^{l_{k+1}}(A_{k+1})\right)\Big| < \varepsilon,\end{aligned} \tag{6.28}$$

for any $l \in \mathbb{N}$. Fix N sufficiently large such that the operators $\sigma^{l_m}(A_m)$ and $\eta_{s_j}(\sigma^{l_{k+1}}(A_{k+1}))$ belong to $\mathcal{U}_N$ for any $m \in \{1, \cdots, k+1\}$ and $j \in \{1, \cdots, q\}$. We can choose l sufficiently large such that $\eta_{\pi^{(l)} \circ s_j}(\sigma^{l_{k+1}}(A_{k+1})) \notin \mathcal{U}_N$ for any $j \in \{1, \cdots, q\}$, which by symmetry of ω implies that

$$\begin{aligned} & \omega\left(\sigma^{l_1}(A_1) \ldots \sigma^{l_k}(A_k)\, \eta_{\pi^{(l)} \circ s_j}\left(\sigma^{l_{k+1}}(A_{k+1})\right)\right) \\ = \;& \omega\left(\sigma^{l_1}(A_1) \ldots \sigma^{l_k}(A_k)\, \sigma^{l_{k+1}}(A_{k+1})\right). \end{aligned}$$

Combined with (6.28) and $\lambda_1 + \cdots + \lambda_q = 1$, it yields

$$\left|\omega\left(\sigma^{l_1}(A_1) \ldots \sigma^{l_k}(A_k)\, \sigma^{l_{k+1}}(A_{k+1})\right) - \omega\left(\sigma^{l_1}(A_1) \ldots \sigma^{l_k}(A_k)\right) \zeta_\omega(A_{k+1})\right| < \varepsilon.$$

Since the equality (6.27) is assumed to be verified at fixed $k \geq 1$, it follows that

$$\left|\omega\left(\sigma^{l_1}(A_1) \ldots \sigma^{l_{k+1}}(A_{k+1})\right) - \zeta_\omega(A_1) \ldots \zeta_\omega(A_{k+1})\right| < \varepsilon,$$

for any $\varepsilon > 0$. In other words, by induction the equality (6.27) is proven for any $k \geq 1$. □

As soon as the upper bound is concerned, we combine Lemma 6.6 with Lemmata 6.7–6.9 to obtain that

$$\limsup_{N\to\infty} \{\mathrm{p}_N(\beta, \mu, \lambda, \gamma)\} \leq \mathrm{p}(\beta, \mu, \lambda, 0, h) + \sup_{\zeta \in E^+_{\mathcal{U}_1}} \left\{\gamma |\zeta(a^*_\uparrow a^*_\downarrow)|^2 - \beta^{-1} S(\zeta_0|\zeta)\right\}. \tag{6.29}$$

Here $E^+_{\mathcal{U}_1}$ denotes the set of even states on the (one–site) algebra $\mathcal{U}_1$. Now the proof of the upper bound (6.2) easily follows from the passivity of Gibbs states on $\mathcal{U}_1$. Indeed, we apply Lemma 6.4 to the one–site Hamiltonians $H_0 = H_1(0)$ (see (2.1)) and

$$H_1 = -\frac{c}{2} a^*_\uparrow a^*_\downarrow - \frac{\bar{c}}{2} a_\uparrow a_\downarrow$$

in order to bound the relative entropy $S(\zeta_0 \,|\, \zeta)$. More precisely, it follows that

$$\begin{aligned} \mathrm{p}(\beta, \mu, \lambda, 0, h) - \beta^{-1} S(\zeta_0 \,|\, \zeta) \;\leq\;& p(c/(2\gamma)) - x \mathrm{Re}\{\zeta(a_\uparrow a_\downarrow)\} \\ & - y\, \mathrm{Im}\{\zeta(a_\uparrow a_\downarrow)\}, \end{aligned} \tag{6.30}$$

for any state $\zeta \in E^+_{\mathcal{U}_1}$ and any $c \in \mathbb{C}$ with $x := \mathrm{Re}\{c\}$ and $y := \mathrm{Im}\{c\}$. Consequently, from (6.29) we deduce that

$$\begin{aligned} \limsup_{N\to\infty} \{\mathrm{p}_N(\beta, \mu, \lambda, \gamma, h)\} \;\leq\;& \sup_{\zeta \in E^+_{\mathcal{U}_1}} \Big\{ \inf_{x,y \in \mathbb{R}} \Big\{ \gamma (\mathrm{Re}\{\zeta(a_\uparrow a_\downarrow)\}^2 + \mathrm{Im}\{\zeta(a_\uparrow a_\downarrow)\}^2) \\ & - x\, \mathrm{Re}\{\zeta(a_\uparrow a_\downarrow)\} - y\, \mathrm{Im}\{\zeta(a_\uparrow a_\downarrow)\} \\ & + p((x+iy)/(2\gamma)) \Big\}\Big\} \\ \leq\;& \sup_{t,s \in \mathbb{R}} \Big\{ \inf_{x,y \in \mathbb{R}} \Big\{ \gamma\left(t^2 + s^2\right) - tx - sy \\ & + p((x+iy)/(2\gamma)) \Big\}\Big\}. \end{aligned}$$

In particular, by fixing $x = 2t\gamma$ and $y = 2s\gamma$ in the infimum we finally obtain

$$\limsup_{N\to\infty} \{\mathrm{p}_N(\beta, \mu, \lambda, \gamma, h)\} \leq \sup_{t,s \in \mathbb{R}} \left\{-\gamma\left(t^2 + s^2\right) + p(t + is)\right\},$$

i.e., the upper bound (6.2) for any $\beta, \gamma > 0$ and $\mu, \lambda, h \in \mathbb{R}$.

6.2 Equilibrium and ground states of the strong coupling BCS-Hubbard model

It follows immediately from the passivity of Gibbs states that

$$\mathrm{p}(\beta, \mu, \lambda, \gamma, h) \geq \Delta(\omega) - \beta^{-1} \tilde{S}(\zeta_0, \omega) + \mathrm{p}(\beta, \mu, \lambda, 0, h), \tag{6.31}$$

for any $\omega \in E_{\mathcal{U}}^{S,+}$, cf. (6.1) and Lemmata 6.3–6.4. Therefore, by using Lemma 6.6 with (6.22) the (infinite volume) pressure can be written as

$$\mathrm{p}\left(\beta,\mu,\lambda,\gamma,h\right)=\sup_{\omega\in E_{\mathcal{U}}^{S,+}}\left\{\Delta\left(\omega\right)-\beta^{-1}\tilde{S}\left(\zeta_{0},\omega\right)\right\}+\mathrm{p}\left(\beta,\mu,\lambda,0,h\right).$$

Moreover, as shown above (see the upper bound in the proof of Lemma 6.6), any weak* limit point ω_∞ of local Gibbs states ω_N (1.6) when $N\to\infty$ satisfies (6.31) with equality.

Indeed, by using (6.13) one obtains for any state ω that

$$\begin{aligned}\frac{1}{N}\left(-\omega\left(\mathrm{H}_{N}\right)-\beta^{-1}S\left(\mathrm{tr}_{N}\left|\omega\right|_{\mathcal{U}_{N}}\right)\right) &= \frac{\gamma}{N^{2}}\sum_{l,m=1}^{N}\omega\left(a_{\kappa(l),\uparrow}^{*}a_{\kappa(l),\downarrow}^{*}a_{\kappa(m),\downarrow}a_{\kappa(m),\uparrow}\right)\\ &\quad -\frac{1}{\beta N}S\left(\omega_{\zeta_{0}}|_{\mathcal{U}_{N}}\left|\omega\right|_{\mathcal{U}_{N}}\right)\\ &\quad +\mathrm{p}_{N}\left(\beta,\mu,\lambda,0,h\right),\end{aligned}\tag{6.32}$$

with p_N being the (finite volume) pressure (1.4) associated with the Hamiltonian H_N (1.2), ω_{ζ_0} being the product state obtained by "copying" the state ζ_0 (6.1) on the one–site algebra $\mathcal{U}_1$ (see (6.7)), and with the trace state tr_N defined on the local algebra $\mathcal{U}_N$ for $N\in\mathbb{N}$ by

$$\mathrm{tr}_{N}(\,\cdot\,):=\frac{\mathrm{Trace}(\,\cdot\,)}{\mathrm{Trace}(\mathbb{I}_{\mathcal{U}_{N}})}.$$

For any permutation invariant state ω it is straightforward to check that the limits

$$\lim_{N\to\infty}\left\{N^{-1}S\left(\omega_{\zeta_{0}}|_{\mathcal{U}_{N}}\left|\omega\right|_{\mathcal{U}_{N}}\right)\right\}$$

and

$$\mathfrak{e}\left(\omega\right):=\lim_{N\to\infty}\left\{N^{-1}\omega\left(\mathrm{H}_{N}\right)\right\}=\omega\left(H_{1}(0)\right)-\Delta\left(\omega\right)$$

exist for any fixed parameters $\beta,\gamma>0$ and $\mu,\lambda,h\in\mathbb{R}$, see respectively (2.1) and Lemma 6.3 for the definitions of $H_1(0)$ and $\Delta(\omega)$. Combined with (6.19) and (6.32) it then follows that the usual entropy density

$$\begin{aligned}\tilde{S}\left(\omega\right):= &\quad -\lim_{N\to\infty}\left\{N^{-1}S\left(\mathrm{tr}_{N}\left|\omega\right|_{\mathcal{U}_{N}}\right)\right\}\\ = &\quad -\lim_{N\to\infty}\left\{\frac{1}{N}\mathrm{Trace}\left(D_{\omega|_{\mathcal{U}_{N}}}\log D_{\omega|_{\mathcal{U}_{N}}}\right)\right\}<\infty\end{aligned}$$

of the permutation invariant state ω also exists and

$$\lim_{N\to\infty}\frac{1}{\beta N}S\left(\omega_{\zeta_{0}}|_{\mathcal{U}_{N}}\left|\omega\right|_{\mathcal{U}_{N}}\right)=\mathfrak{e}(\omega)+\Delta(\omega)-\beta^{-1}\tilde{S}\left(\omega\right)+p(\beta,\mu,\lambda,0,h).$$

The set $\mathit{\Omega}_\beta=\mathit{\Omega}_\beta(\mu,\lambda,\gamma,h)$ of *equilibrium states* of the strong coupling BCS–Hubbard model is defined by

$$\begin{aligned}\mathit{\Omega}_{\beta}:= &\quad \Big\{\omega\in E_{\mathcal{U}}^{S,+}:-\mathfrak{e}\left(\omega\right)+\beta^{-1}\tilde{S}\left(\omega\right)=\mathrm{p}\left(\beta,\mu,\lambda,\gamma,h\right)\\ &\qquad =\Delta\left(\omega\right)-\beta^{-1}\tilde{S}\left(\zeta_{0},\omega\right)+\mathrm{p}\left(\beta,\mu,\lambda,0,h\right)\Big\}.\end{aligned}$$

Note that $\mathit{\Omega}_\beta$ contains per construction all weak* limit points of local Gibbs states ω_N as $N\to\infty$.

Consequently, the equilibrium states are, as usual, the minimizers of the free energy functional

$$\omega\mapsto\mathfrak{F}(\omega):=\mathfrak{e}(\omega)-\beta^{-1}\tilde{S}(\omega)\tag{6.33}$$

on the convex and weak*–compact set $E_{\mathcal{U}}^{S,+}$, cf. (1.5). They also maximize the upper semicontinuous affine functional $\omega\mapsto\Delta(\omega)-\beta^{-1}\tilde{S}(\zeta_0,\omega)$. It follows that $\mathit{\Omega}_\beta$ is a closed face of $E_{\mathcal{U}}^{S,+}$ and we have in this set a notion of pure and mixed thermodynamic phases (equilibrium states) by identifying purity with extremality. In particular, it is convex and weak*–compact. Each weak*–limit ω of equilibrium states $\omega^{(n)} \in \Omega_{\beta_n}(\mu_n, \lambda_n, \gamma_n, h_n)$ such that $(\mu_n, \lambda_n, \gamma_n, h_n) \to (\mu, \lambda, \gamma, h)$ and $\beta_n \to \infty$ is called a *ground state* of the strong coupling BCS–Hubbard model. The set of all ground states with parameters $\gamma > 0$ and $\mu, \lambda, h \in \mathbb{R}$ is denoted by $\Omega_\infty = \Omega_\infty(\mu, \lambda, \gamma, h)$. Extremal states of the weak*–compact convex set Ω_∞ are called *pure* ground states.

We analyze now the set of pure equilibrium states, i.e., the equilibrium states $\omega \in \Omega_\beta$ belonging to the set $\mathcal{E}_{\mathcal{U}}^{S,+}$ of extremal points of $E_{\mathcal{U}}^{S,+}$, cf. (6.22). First, from Lemmata 6.7–6.9 recall that any extremal state is a product state ω_ζ (6.7), i.e., it is obtained by "copying" a state ζ on the one–site algebra $\mathcal{U}_1$ to the other sites. In particular, by combining (6.22) with (6.31) observe that

$$\mathrm{p}\,(\beta, \mu, \lambda, \gamma, h) = \sup_{\zeta \in E_{\mathcal{U}_1}^+} \left\{ \gamma |\zeta(a_\uparrow^* a_\downarrow^*)|^2 - \beta^{-1} S(\zeta_0|\zeta) \right\} + \mathrm{p}\,(\beta, \mu, \lambda, 0, h)\,. \tag{6.34}$$

Therefore, a product state ω_ζ is a pure equilibrium state if and only if ζ belongs to the set $\mathcal{G}_\beta = \mathcal{G}_\beta(\mu, \lambda, \gamma, h)$ of one–site equilibrium states defined by

$$\mathcal{G}_\beta := \left\{ \zeta \in E_{\mathcal{U}_1}^+ : \gamma |\zeta(a_\uparrow^* a_\downarrow^*)|^2 - \beta^{-1} S(\zeta_0|\zeta) = \mathrm{p}\,(\beta, \mu, \lambda, \gamma, h) - \mathrm{p}\,(\beta, \mu, \lambda, 0, h) \right\}. \tag{6.35}$$

In other words, the study of pure states of Ω_β can be reduced, without loss of generality, to the analysis of $\mathcal{G}_\beta$. The first important statement concerns the characterization of the set $\mathcal{G}_\beta$ in relation with the variational problems (2.4) and (6.34).

Theorem 6.10 (Explicit description of one-site equilibrium states)
For any $\beta, \gamma > 0$ and $\mu, \lambda, h \in \mathbb{R}$, the set $\mathcal{G}_\beta$ of one–site equilibrium states are given by the states ζ_{c_β} (6.1) with $\mathrm{c}_\beta := \mathrm{r}_\beta^{1/2} e^{i\phi}$ for any order parameter r_β solution of (2.4) and any phase $\phi \in [0, 2\pi)$.

Proof: Take any solution r_β of (2.4) and any $\phi \in [0, 2\pi)$. Then, from (6.14) observe that

$$-\beta^{-1} S(\zeta_0 \,|\, \zeta_{\mathrm{c}_\beta}) + \mathrm{p}\,(\beta, \mu, \lambda, 0, h) = -\gamma \zeta_{\mathrm{c}_\beta}(\mathrm{c}_\beta a_\uparrow^* a_\downarrow^* + \bar{\mathrm{c}}_\beta a_\downarrow a_\uparrow) + p(\mathrm{c}_\beta). \tag{6.36}$$

Since $\zeta_{\mathrm{c}_\beta}(a_\downarrow a_\uparrow) = \mathrm{c}_\beta$ and $\zeta_{\mathrm{c}_\beta}(a_\uparrow^* a_\downarrow^*) = \bar{\mathrm{c}}_\beta$, the last equality combined with Theorem 2.1 implies that

$$\gamma |\zeta_{\mathrm{c}_\beta}(a_\downarrow a_\uparrow)|^2 - \beta^{-1} S(\zeta_0 \,|\, \zeta_{\mathrm{c}_\beta}) = \mathrm{p}\,(\beta, \mu, \lambda, \gamma, h) - \mathrm{p}\,(\beta, \mu, \lambda, 0, h)\,. \tag{6.37}$$

In other words, ζ_{c_β} is a maximizer of the variational problem defined in (6.34) and hence, $\zeta_{\mathrm{c}_\beta} \in \mathcal{G}_\beta$.

On the other hand, any state $\zeta \in \mathcal{G}_\beta$ satisfies (6.37) and by combining Theorem 2.1 with the inequality (6.30) for $c = 2\gamma\zeta(a_\downarrow a_\uparrow)$ it follows that

$$-\gamma |\zeta(a_\downarrow a_\uparrow)|^2 + p(\zeta(a_\downarrow a_\uparrow)) \geq \sup_{c \in \mathbb{C}} \{-\gamma |c|^2 + p(c)\}.$$

Hence, $\zeta(a_\downarrow a_\uparrow) = \mathrm{r}_\beta^{1/2} e^{i\phi} = \mathrm{c}_\beta$ for some $\phi \in [0, 2\pi)$. It remains to prove that the equality $\zeta(a_\downarrow a_\uparrow) = \mathrm{c}_\beta$ uniquely defines the one–site equilibrium state $\zeta \in \mathcal{G}_\beta$. It follows from $\zeta(a_\downarrow a_\uparrow) = \zeta_{\mathrm{c}_\beta}(a_\downarrow a_\uparrow) = \mathrm{c}_\beta$ with $\zeta, \zeta_{\mathrm{c}_\beta} \in \mathcal{G}_\beta$ that $S(\zeta_0|\zeta_{\mathrm{c}_\beta}) = S(\zeta_0|\zeta)$ and

$$\gamma \zeta(\mathrm{c}_\beta a_\uparrow^* a_\downarrow^* + \bar{\mathrm{c}}_\beta a_\downarrow a_\uparrow) - \beta^{-1} S(\zeta_0|\zeta) = P^{H_1(\mathrm{c}_\beta)} - P^{H_1(0)} \tag{6.38}$$

because of (6.36), see (2.1) for the definition of $H_1(c)$. By Lemma 6.4, one obtains for any self–adjoint $A \in \mathcal{U}_1$ that

$$-\zeta(A) + \gamma \zeta(\mathrm{c}_\beta a_\uparrow^* a_\downarrow^* + \bar{\mathrm{c}}_\beta a_\downarrow a_\uparrow) - \beta^{-1} S(\zeta_0|\zeta) \leq P^{H_1(\mathrm{c}_\beta)+A} - P^{H_1(0)}. \tag{6.39}$$

Consequently, we obtain by combining (6.38) and (6.39) that

$$P^{H_1(\mathrm{c}_\beta)+A} - P^{H_1(\mathrm{c}_\beta)} \geq -\zeta(A),$$

for any self–adjoint $A \in \mathcal{U}_1$ and $\zeta \in \mathcal{G}_\beta$ such that $\zeta(a_\downarrow a_\uparrow) = \mathrm{c}_\beta$. In other words, the functional $\{-\zeta\}$ is tangent to the pressure at $H_1(\mathrm{c}_\beta)$. Since the convex map $A \mapsto P^{H_1(\mathrm{c}_\beta)+A}$ is continuously differentiable and self–adjoint elements separate states, the tangent functional is unique and $\zeta = \zeta_{\mathrm{c}_\beta}$. $\square$

It follows immediately from the theorem above that pure states of Ω_β solve the gap equation:

Corollary 6.11 (Gap equation for pure equilibrium states)
For any $\beta,\gamma>0$ and $\mu,\lambda,h\in\mathbb{R}$, pure states from Ω_β are precisely the product states $\omega_{\zeta_{\mathrm{c}_\beta}}$ satisfying the gap equation $\omega_{\zeta_{\mathrm{c}_\beta}}(a_{\kappa(l),\uparrow},a_{\kappa(l),\downarrow})=\mathrm{c}_\beta$ for any $l\in\mathbb{N}$ and with $\mathrm{c}_\beta:=\mathrm{r}_\beta^{1/2}e^{i\phi}$ being any maximizer of the first variational problem given in Theorem 2.1.

If $\mathrm{c}_\beta\neq0$, observe that the gap equation $\omega_{\zeta_{\mathrm{c}_\beta}}(a_{\kappa(l),\uparrow},a_{\kappa(l),\downarrow})=\mathrm{c}_\beta$ with ζ_c defined in (6.1) corresponds to the Euler–Lagrange equation satisfied by the solutions $\mathrm{c}_\beta:=\mathrm{r}_\beta^{1/2}e^{i\phi}$ of the first variational problem given in Theorem 2.1. The phase $\phi\in[0,2\pi)$ is arbitrarily taken because of the gauge invariance of the map $c\mapsto p(c)$, and the gap equation $\omega_{\zeta_{\mathrm{c}_\beta}}(a_{\kappa(l),\uparrow},a_{\kappa(l),\downarrow})=\mathrm{c}_\beta$ can be reduced to (2.5). In other words, if $\mathrm{c}_\beta\neq0$, the gap equation can be written in two different ways: either $\omega_{\zeta_{\mathrm{c}_\beta}}(a_{\kappa(l),\uparrow},a_{\kappa(l),\downarrow})=\mathrm{c}_\beta$ in the view point of extremal equilibrium states or (2.5) in the view point of the order parameter r_β.

From this last corollary observe also that the existence of non–zero maximizers $\mathrm{c}_\beta\neq0$ implies the existence of equilibrium states breaking the $U(1)$–gauge symmetry satisfied by H_N (1.2). This breakdown of the $U(1)$–gauge symmetry for $\mathrm{c}_\beta\neq0$ is already explained by Theorem 3.3, which can be proven by our notion of equilibrium states as follows.

Consider the upper semicontinuous convex map on $E_{\mathcal{U}}^{S,+}$ defined for any $\alpha\geq0$ and $\phi\in[0,2\pi)$ by

$$\omega\mapsto-\mathfrak{e}\left(\omega\right)+\beta^{-1}\tilde{S}\left(\omega\right)+2\alpha\,\mathrm{Re}\left\{e^{i\phi}\omega\left(a_{\downarrow}^{*}a_{\uparrow}^{*}\right)\right\}. \tag{6.40}$$

From Section 6.1 it is straightforward to check that

$$\begin{aligned}\mathrm{p}_{\alpha,\phi}\left(\beta,\mu,\lambda,\gamma,h\right) &:= \lim_{N\rightarrow\infty}\left\{\frac{1}{\beta N}\ln\mathrm{Trace}\left(e^{-\beta\mathrm{H}_{N,\alpha,\phi}}\right)\right\}\\ &= \sup_{\omega\in E_{\mathcal{U}}^{S,+}}\left\{-\mathfrak{e}\left(\omega\right)+\beta^{-1}\tilde{S}\left(\omega\right)+2\alpha\,\mathrm{Re}\left\{e^{i\phi}\omega\left(a_{\downarrow}^{*}a_{\uparrow}^{*}\right)\right\}\right\},\end{aligned} \tag{6.41}$$

with the Hamiltonian $\mathrm{H}_{N,\alpha,\phi}$ defined in (3.1). Moreover, any weak*–limits $\omega_{\infty,\alpha,\phi}$ of local Gibbs states

$$\omega_{N,\alpha,\phi}\left(\cdot\right):=\frac{\mathrm{Trace}\left(\;\cdot\;e^{-\beta\mathrm{H}_{N,\alpha,\phi}}\right)}{\mathrm{Trace}\left(e^{-\beta\mathrm{H}_{N,\alpha,\phi}}\right)} \tag{6.42}$$

are equilibrium states (see the proof of Lemma 6.6 applied to $\mathrm{H}_{N,\alpha,\phi}$), i.e., the state $\omega_{\infty,\alpha,\phi}$ belongs to the (non-empty) convex set $\Omega_{\beta,\alpha,\phi}=\Omega_{\beta,\alpha,\phi}(\mu,\lambda,\gamma,h)$ of maximizers of (6.40) at fixed $\alpha\geq0$ and $\phi\in[0,2\pi)$. In fact, one gets the following statement, which implies Theorem 3.3.

Theorem 6.12 (Breakdown of the $U(1)$-gauge symmetry)
Take $\beta,\gamma>0$ and real numbers μ,λ,h away from any critical point. Then at fixed phase $\phi\in[0,2\pi)$,

$$\lim_{\alpha\downarrow0}\lim_{N\rightarrow\infty}\frac{1}{N}\sum_{l=1}^{N}\omega_{N,\alpha,\phi}\left(a_{\kappa(l),\downarrow}a_{\kappa(l),\uparrow}\right)=\lim_{\alpha\downarrow0}\omega_{\infty,\alpha,\phi}(a_{\kappa(1),\downarrow}a_{\kappa(1),\uparrow})=\mathrm{r}_\beta^{1/2}e^{i\phi},$$

with $\omega_{\infty,\alpha,\phi}\in\Omega_{\beta,\alpha,\phi}$ being the unique maximizer of (6.40) for sufficiently small $\alpha\geq0$.

Proof: First we need to characterize pure states of $\Omega_{\beta,\alpha,\phi}$ as it is done in Corollary 6.11 for $\alpha=0$. By convexity and upper semicontinuity, note that maximizers of (6.40) are taken on the set of extremal states whereas the set of extremal maximizers is a face. Since extremal states are product states (cf. Lemma 6.7-6.9), we get that

$$\begin{aligned}&\sup_{\omega\in E_{\mathcal{U}}^{S,+}}\left\{-\mathfrak{e}\left(\omega\right)+\beta^{-1}\tilde{S}\left(\omega\right)+\alpha\,\mathrm{Re}\left\{e^{i\phi}\omega\left(a_{\downarrow}^{*}a_{\uparrow}^{*}\right)\right\}\right\}\\ =\;&\sup_{c\in\mathbb{C}}\left\{-\gamma|c|^{2}+p\left(c+\alpha\gamma^{-1}e^{i\phi}\right)\right\},\end{aligned} \tag{6.43}$$

as in the case $\alpha = 0$ (see (2.3) for the definition of $p(c)$). If $\mathrm{c}_{\beta,\alpha,\phi} = \mathrm{c}_{\beta,\alpha,\phi}(\mu, \lambda, \gamma, h) \in \mathbb{C}$ is a maximizer of

$$-\gamma|c|^2 + p(c + \alpha\gamma^{-1}e^{i\phi}), \tag{6.44}$$

then observe that $z_{\beta,\alpha,\phi} := \mathrm{c}_{\beta,\alpha,\phi} + \alpha\gamma^{-1}e^{i\phi}$ maximizes the function

$$-\gamma|z - \alpha\gamma^{-1}e^{i\phi}|^2 + p(z)$$

of the complex variable $z \in \mathbb{C}$. By gauge invariance of the map $z \mapsto p(\beta, \mu, \lambda, h; z)$, it follows that $z_{\beta,\alpha,\phi} \in e^{i\phi}\mathbb{R}$ and thus $\mathrm{c}_{\beta,\alpha,\phi} \in e^{i\phi}\mathbb{R}$. Using this, we extend Corollary 6.11 to $\alpha \geq 0$ and $\phi \in [0, 2\pi)$. In other words, for any $\beta, \gamma > 0$, $\alpha \geq 0$, $\phi \in [0, 2\pi)$ and $\mu, \lambda, h \in \mathbb{R}$, pure states of $\mathit{\Omega}_{\beta,\alpha,\phi}$ are product states $\omega_{\zeta_{\mathrm{c}_{\beta,\alpha,\phi}}}$ satisfying the gap equation

$$\omega_{\zeta_{\mathrm{c}_{\beta,\alpha,\phi}}}(a_{\kappa(l),\uparrow}, a_{\kappa(l),\downarrow}) = \mathrm{c}_{\beta,\alpha,\phi}, \tag{6.45}$$

for any $l \in \mathbb{N}$ and with $\mathrm{c}_{\beta,\alpha,\phi} \in e^{i\phi}\mathbb{R}$ being any maximizer of (6.44).

As $|c| \to \infty$, notice that $p(c) = \mathcal{O}(|c|)$. So, by gauge invariance we obtain

$$\begin{aligned} \sup_{c\in\mathbb{C}}\{-\gamma|c|^2 + p(c + \alpha\gamma^{-1}e^{i\phi})\} &= \max_{s\in[-M,M]}\left\{-\gamma|s\, e^{i\phi}|^2 + p\left([s + \alpha\gamma^{-1}]e^{i\phi}\right)\right\} \\ &= \max_{s\in[-M,M]}\{-\gamma s^2 + p(s + \alpha\gamma^{-1})\}, \end{aligned}$$

for any $\alpha \in (0, 1)$ and $M < \infty$ sufficiently large. Consequently, if the parameters β, μ, λ, γ, and h are such that the maximizer r_β (2.4) is unique, then the maximizer $\mathrm{c}_{\beta,\alpha,\phi} \in e^{i\phi}\mathbb{R}$ of (6.44) is also unique as soon as $\alpha > 0$ is sufficiently small. Indeed the map $s \mapsto p(s)$ is continuous on the compact interval $[-M, M]$. In particular, from (6.45) there is a unique maximizer of (6.40), i.e.,

$$\mathit{\Omega}_{\beta,\alpha,\phi} = \{\omega_{\zeta_{\mathrm{c}_{\beta,\alpha,\phi}}}\}. \tag{6.46}$$

Moreover, $\mathrm{c}_{\beta,\alpha,\phi}$ converges to $\mathrm{r}_\beta^{1/2}e^{i\phi}$ as $\alpha \to 0$. Therefore, it follows from (6.45) that

$$\lim_{\alpha\downarrow 0}\omega_{\zeta_{\mathrm{c}_{\beta,\alpha,\phi}}}\left(a_{\kappa(l),\downarrow}a_{\kappa(l),\uparrow}\right) = \mathrm{r}_\beta^{1/2}e^{i\phi} \tag{6.47}$$

for any $l \in \mathbb{N}$.

By permutation invariance

$$\frac{1}{N}\sum_{l=1}^{N}\omega_{N,\alpha,\phi}\left(a^*_{\kappa(l),\uparrow}a^*_{\kappa(l),\downarrow}\right) = \omega_{N,\alpha,\phi}\left(a^*_{\kappa(1),\uparrow}a^*_{\kappa(1),\downarrow}\right).$$

Now, let $\{N_j^{(1)}\}$ and $\{N_j^{(2)}\}$ be two subsequences in $\mathbb{N}$ such that

$$\begin{aligned} \lim_{j\to\infty}\omega_{N_j^{(1)},\alpha,\phi}\left(a^*_{\kappa(1),\uparrow}a^*_{\kappa(1),\downarrow}\right) &= \limsup_{N\to\infty}\omega_{N,\alpha,\phi}\left(a^*_{\kappa(1),\uparrow}a^*_{\kappa(1),\downarrow}\right), \\ \lim_{j\to\infty}\omega_{N_j^{(2)},\alpha,\phi}\left(a^*_{\kappa(1),\uparrow}a^*_{\kappa(1),\downarrow}\right) &= \liminf_{N\to\infty}\omega_{N,\alpha,\phi}\left(a^*_{\kappa(1),\uparrow}a^*_{\kappa(1),\downarrow}\right). \end{aligned}$$

We can assume without loss of generality that $\omega_{N_j^{(2)}}$ and $\omega_{N_j^{(1)}}$ both converge w.r.t. the weak*–topology as $j \to \infty$. Since any weak*–limits $\omega_{\infty,\alpha,\phi}$ of local Gibbs states $\omega_{N,\alpha,\phi}$ (6.42) are equilibrium states (see again the proof of Lemma 6.6), i.e., $\omega_{\infty,\alpha,\phi} \in \mathit{\Omega}_{\beta,\alpha,\phi}$, the theorem then follows from (6.46) and (6.47). Indeed, for any $\beta, \gamma > 0$ and $\mu, \lambda, h \in \mathbb{R}$ away from any critical point, the sequence $\omega_{N,\alpha,\phi}$ of local Gibbs state converges towards $\omega_{\infty,\alpha,\phi} = \omega_{\zeta_{\mathrm{c}_{\beta,\alpha,\phi}}}$ in the weak*–topology as soon as $\alpha \geq 0$ is sufficiently small. $\square$

From Corollary 6.11 note that the expectation values of Cooper fields

$$\begin{aligned} \Phi_{\kappa(l)} &:= a^*_{\kappa(l),\downarrow}a^*_{\kappa(l),\uparrow} + a_{\kappa(l),\uparrow}a_{\kappa(l),\downarrow} \\ \Psi_{\kappa(l)} &:= i(a^*_{\kappa(l),\downarrow}a^*_{\kappa(l),\uparrow} - a_{\kappa(l),\uparrow}a_{\kappa(l),\downarrow}) \end{aligned} \tag{6.48}$$

are

$$\omega_{\zeta_{\mathrm{c}_\beta}}(\Phi_{\kappa(l)}) = 2\,\mathrm{Re}\{\mathrm{c}_\beta\} \text{ and } \omega_{\zeta_{\mathrm{c}_\beta}}(\Psi_{\kappa(l)}) = 2\,\mathrm{Im}\{\mathrm{c}_\beta\} \tag{6.49}$$

for any pure state $\omega_{\zeta_{\mathrm{c}_\beta}}$ of Ω_β and $l \in \mathbb{N}$, where we recall that $\mathrm{c}_\beta := \mathrm{r}_\beta^{1/2} e^{i\phi}$ is some maximizer of the first variational problem given in Theorem 2.1. In particular, $\omega(\Phi_{\kappa(l)}) \neq 0$ or $\omega(\Psi_{\kappa(l)}) \neq 0$ for any pure state $\omega \in \Omega_\beta$ is a manifestation of the breakdown of the $U(1)$–gauge symmetry.

Unfortunately, the operators $\Phi_{\kappa(l)}$ and $\Psi_{\kappa(l)}$ do not correspond to any experiment, as they are not gauge invariant. More generally, experiments only "see" the restriction of states $\omega_{\zeta_{\mathrm{c}_\beta}}$ to the subalgebra of gauge invariant elements. Consequently, the next step is to prove the so–called *off diagonal long range order* (ODLRO) property proposed by Yang [38] to define the superconducting phase. Indeed, one detects the presence of $U(1)$–gauge symmetry breaking by considering the asymptotics, as $|l-m| \to \infty$, of the ($U(1)$–gauge symmetric) Cooper pair correlation function

$$G_\omega(l,m) := \omega(a_{\kappa(l),\uparrow}^* a_{\kappa(l),\downarrow}^* a_{\kappa(m),\downarrow} a_{\kappa(m),\uparrow}) \tag{6.50}$$

associated with some state ω. In particular, if $G_\omega(l,m)$ converges to some fixed non–zero value whenever $|l-m| \to \infty$, the state ω shows *off diagonal long range order* (ODLRO). This property can directly be analyzed for equilibrium states from our next statement.

Theorem 6.13 (Cooper pair correlation function)
For any $\beta, \gamma > 0$ and $\mu, \lambda, h \in \mathbb{R}$ away from any critical point, the Cooper pair correlation function $G_{\omega_N}(l,m)$ associated with the local Gibbs state ω_N converges for fixed $l \neq m$ towards

$$\lim_{N\to\infty} G_{\omega_N}(l,m) = G_\omega(l,m) = \mathrm{r}_\beta,$$

for any equilibrium state $\omega \in \Omega_\beta$, and with r_β being the solution of (2.4).

Proof: By similar arguments as in the proof of Theorem 6.12, if $G_\omega(l,m) = \mathrm{r}_\beta$ for all equilibrium states ω, then

$$\lim_{N\to\infty} G_{\omega_N}(l,m) = \mathrm{r}_\beta.$$

By permutation invariance of $\omega \in \Omega_\beta$, note that

$$G_\omega(l,m) = G_\omega(1,2) \tag{6.51}$$

for any $l \neq m$. If $\omega = \omega_{\zeta_{\mathrm{c}_\beta}}$ is an extremal equilibrium state, then one clearly has

$$G_{\omega_{\zeta_{\mathrm{c}_\beta}}}(1,2) = \zeta_{\mathrm{c}_\beta}(a_\uparrow^* a_\downarrow^*)\zeta_{\mathrm{c}_\beta}(a_\downarrow a_\uparrow) = |\mathrm{c}_\beta|^2 = \mathrm{r}_\beta.$$

On the other hand, the set Ω_β of equilibrium states for fixed parameters $\beta, \gamma > 0$, and $\mu, \lambda, h \in \mathbb{R}$ is weak*–compact. In particular, if $\omega \in \Omega_\beta$ is not extremal, the function $G_\omega(1,2)$ is given, up to arbitrarily small errors, by convex sums of the form

$$\sum_{j=1}^{k} \lambda_j G_{\omega^{(j)}}(1,2), \quad \lambda_1, \ldots, \lambda_k \geq 0, \quad \lambda_1 + \ldots + \lambda_k = 1, \tag{6.52}$$

where $\{\omega^{(j)}\}_{j=1,\ldots,k}$ are extremal equilibrium states. Since any weak*–limit ω_∞ of local Gibbs states ω_N (1.6) is an equilibrium state (see proof of Lemma 6.6), the theorem is then a consequence of (6.51)–(6.52). □

Since

$$\begin{aligned} & \frac{1}{N^2}\sum_{l,m=1}^{N} \omega_N\left(a_{\kappa(l),\uparrow}^* a_{\kappa(l),\downarrow}^* a_{\kappa(m),\downarrow} a_{\kappa(m),\uparrow}\right) \\ = \ & \frac{N(N-1)}{N^2}\omega_N\left(a_{\kappa(1),\uparrow}^* a_{\kappa(1),\downarrow}^* a_{\kappa(2),\downarrow} a_{\kappa(2),\uparrow}\right) + \mathcal{O}(N^{-1}), \end{aligned}$$

note that this theorem implies Theorem 3.1.

Therefore, away from any critical point, if an equilibrium state shows ODLRO then all pure equilibrium states break the $U(1)$–gauge symmetry. Conversely, if all pure equilibrium states break the $U(1)$–gauge symmetry, then all equilibrium state show ODLRO. This is due to the fact that the order parameter r_β is unique away from any critical point. In particular, from Section 7, at sufficiently small inverse temperature β there is no ODLRO and $\Omega_\beta = \{\omega_{\zeta_0}\}$, whereas for sufficiently large β and γ all equilibrium states show ODLRO.

For any $\beta, \gamma > 0$ and real numbers μ, λ, h at some critical point, this property is not satisfied in general. There are indeed cases where the phase transition is of first order, cf. figure 3. In this situation, 0 and some $\mathrm{r}_\beta > 0$ are maximizers at the same time, and hence, there are some equilibrium states breaking the $U(1)$–gauge symmetry and other equilibrium states which do not show ODLRO in this specific situation.

Observe now that the superconducting phase is not only characterized by ODLRO and the breakdown of the $U(1)$–gauge symmetry. Indeed, the two–point correlation function determines its type: s–wave, d–wave, p–wave, etc. In fact, for any extremal equilibrium state $\omega = \omega_{\zeta_{\mathrm{c}_\beta}}$, $x, y \in \mathbb{Z}^d$ and $s_1, s_2 \in \{\uparrow, \downarrow\}$, one clearly has

$$\omega_{\zeta_{\mathrm{c}_\beta}}(a_{x,s_1} a_{y,s_2}) = \begin{cases} \zeta_{\mathrm{c}_\beta}(a_{x,s_1})\zeta_{\mathrm{c}_\beta}(a_{y,s_2}) & \text{if } x \neq y \\ \zeta_{\mathrm{c}_\beta}(a_{x,s_1} a_{x,s_2}) & \text{if } x = y \end{cases} = \begin{cases} 0 & \text{if } x \neq y. \\ 0 & \text{if } x = y,\ s_1 = s_2. \\ \mathrm{c}_\beta & \text{if } x = y,\ s_1 \neq s_2. \end{cases}$$

As a consequence, for any equilibrium state $\omega \in \Omega_\beta$, we have $\omega(a_{x,s_1} a_{y,s_2}) = \omega(a_{0,s_1} a_{0,s_2})\delta_{x,y}$ and we obtain a *s–wave* superconducting phase. In particular, Theorem 3.4 is a simple consequence of this last equalities combined with (6.46), (6.47) and the fact that any weak*–limits $\omega_{\infty,\alpha,\phi} \in \Omega_{\beta,\alpha,\phi}$ of local Gibbs states $\omega_{N,\alpha,\phi}$ (6.42) are equilibrium states (see again the proof of Lemma 6.6).

Now we would like to pursue this analysis of equilibrium states by showing that their definition is in accordance with results of Theorems 3.8, 3.10 and 3.12. This statement is given in the next theorem.

Theorem 6.14 (Uniqueness of densities for equilibrium states)
Take $\beta, \gamma > 0$ and real numbers μ, λ, h away from any critical point. Then, for any equilibrium state $\omega \in \Omega_\beta$ and $l \in \mathbb{N}$, all densities are uniquely defined:
(i) The electron density is equal to

$$\lim_{N\to\infty} \left\{ \frac{1}{N} \sum_{l'=1}^{N} \omega_N \left(n_{\kappa(l'),\uparrow} + n_{\kappa(l'),\downarrow} \right) \right\} = \omega(n_{\kappa(l),\uparrow} + n_{\kappa(l),\downarrow}) = \mathrm{d}_\beta,$$

cf. Theorem 3.8.
(ii) The magnetization density is equal to

$$\lim_{N\to\infty} \left\{ \frac{1}{N} \sum_{l'=1}^{N} \omega_N \left(n_{\kappa(l'),\uparrow} - n_{\kappa(l'),\downarrow} \right) \right\} = \omega(n_{\kappa(l),\uparrow} - n_{\kappa(l),\downarrow}) = \mathrm{m}_\beta,$$

cf. Theorem 3.10.
(iii) The Coulomb correlation density is equal to

$$\lim_{N\to\infty} \left\{ \frac{1}{N} \sum_{l'=1}^{N} \omega_N \left(n_{\kappa(l'),\uparrow} n_{\kappa(l'),\downarrow} \right) \right\} = \omega(n_{\kappa(l),\uparrow} n_{\kappa(l),\downarrow}) = \mathrm{w}_\beta,$$

cf. Theorem 3.12.

Proof: Suppose first that $\omega \in \Omega_\beta$ is pure. Then, from Corollary 6.11 it follows that

$$\omega \left(n_{\kappa(l),\uparrow} + n_{\kappa(l),\downarrow} \right) = \omega_{\zeta_{\mathrm{c}_\beta}} \left(n_{\kappa(l),\uparrow} + n_{\kappa(l),\downarrow} \right),$$

with $\mathrm{c}_\beta = \mathrm{r}_\beta^{1/2} e^{i\phi}$ for some $\phi \in [0, 2\pi)$. Thus, by using the gauge invariance of the map $c \mapsto p(c)$ we directly get

$$\omega \left(n_{\kappa(l),\uparrow} + n_{\kappa(l),\downarrow} \right) = \partial_\mu p(\beta, \mu, \lambda, \gamma, h; \mathrm{c}_\beta) = \partial_\mu p(\beta, \mu, \lambda, \gamma, h; \mathrm{r}_\beta^{1/2}) = \mathrm{d}_\beta. \tag{6.53}$$

At fixed parameters $\beta, \gamma > 0$, $\mu, \lambda, h \in \mathbb{R}$, recall that the set Ω_β of equilibrium states is weak*–compact. In particular, if $\omega \in \Omega_\beta$ is not pure, it is the weak*–limit of convex combinations of pure states. Therefore, we obtain (6.53) for any $\omega \in \Omega_\beta$. Similarly one gets

$$\omega(n_{\kappa(l),\uparrow} - n_{\kappa(l),\downarrow}) = \mathrm{m}_\beta \quad \text{and} \quad \omega(n_{\kappa(l),\uparrow} n_{\kappa(l),\downarrow}) = \mathrm{w}_\beta, \tag{6.54}$$

for any equilibrium state $\omega \in \Omega_\beta$ and $l \in \mathbb{N}$. Moreover, since any weak*–limit ω_∞ of local Gibbs states ω_N (1.6) is an equilibrium state, i.e., $\omega_\infty \in \Omega_\beta$, we therefore deduce from (6.53)-(6.54), exactly as in the proof of Theorem 6.12, the existence of the limits in the statements (i)-(iii). □

Observe that the weak*–limit $\omega_\infty \in \Omega_\beta$ of local Gibbs states ω_N (1.6) can easily be performed, *even at critical points*, by using the decomposition theory for states [32]:

Theorem 6.15 (Asymptotics of the local Gibbs state ω_N as $N \to \infty$)
Recall that for any $\phi \in [0, 2\pi)$, $\mathrm{c}_\beta := \mathrm{r}_\beta^{1/2} e^{i\phi}$ is a maximizer of the first variational problem given in Theorem 2.1, whereas the states ζ_c and ω_ζ are respectively defined by (6.1) and (6.7). Take any $\beta, \gamma > 0$, $\mu, \lambda, h \in \mathbb{R}$, and let $N \to \infty$.
(i) Away From any critical point, the local Gibbs state ω_N converges in the weak–topology towards the equilibrium state*

$$\omega_\infty(\cdot) = \frac{1}{2\pi} \int_0^{2\pi} \omega_{\zeta_{\mathrm{c}_\beta}}(\cdot)\, \mathrm{d}\phi. \tag{6.55}$$

(ii) For each weak limit point ω_∞ of local Gibbs states ω_N with parameters $(\beta_N, \gamma_N, \mu_N, \lambda_N, h_N)$ converging to any critical point $(\beta, \gamma, \mu, \lambda, h) \in \partial\mathcal{S}$ (2.7), there is $\tau \in [0, 1]$ such that*

$$\omega_\infty(\cdot) = (1 - \tau)\, \omega_{\zeta_0}(\cdot) + \frac{\tau}{2\pi} \int_0^{2\pi} \omega_{\zeta_{\mathrm{c}_\beta}}(\cdot)\, \mathrm{d}\phi.$$

Proof: By $U(1)$–gauge symmetry of the Hamiltonians H_N (1.2) recall that any weak*–limit ω_∞ of local Gibbs states ω_N (1.6) is a $U(1)$–invariant equilibrium state. So, in order to prove the first part of the Theorem it suffices to show that the equilibrium state given in (i) is the unique $U(1)$–invariant state in Ω_β. If the solution r_β of (2.4) is zero, then this follows immediately from Corollary 6.11.

Let $\mathrm{r}_\beta > 0$ be the unique maximizer of (2.4), i.e., $\mathrm{c}_\beta := \mathrm{r}_\beta^{1/2} e^{i\phi} \neq 0$ for any $\phi \in [0, 2\pi)$. Let

$$\partial\Omega_\beta = \{\omega_\zeta : \zeta \in \mathcal{G}_\beta\}$$

be the set of all extremal states of Ω_β, see (6.35) for the definition of the set $\mathcal{G}_\beta$ of one–site equilibrium states. Observe that the closed convex hull of $\partial\Omega_\beta$ is precisely Ω_β and that $\partial\Omega_\beta$ is the image of the torus $[0, 2\pi)$ under the continuous map $\phi \mapsto \omega_{\zeta_{\mathrm{c}_\beta}}$, with $\mathrm{c}_\beta := \mathrm{r}_\beta^{1/2} e^{i\phi}$. This last map defines a homeomorphism between the torus and $\partial\Omega_\beta$. In particular, the set $\partial\Omega_\beta$ is compact and for each equilibrium state $\omega \in \Omega_\beta$ there is a uniquely defined probability measure $\mathrm{d}\hat{\mathfrak{m}}_\omega$ on the torus such that

$$\omega(A) = \int_0^{2\pi} \omega_{\zeta_{\mathrm{c}_\beta}}(A)\, \mathrm{d}\hat{\mathfrak{m}}_\omega(\phi), \text{ for all } A \in \mathcal{U}. \tag{6.56}$$

See, e.g., Proposition 1.2 of [41]. By $U(1)$–invariance of ω_∞, for any $n \in \mathbb{N}$ one has from (6.56) that

$$\omega_\infty\left(\prod_{l=1}^{n} a_{\kappa(l),\uparrow} a_{\kappa(l),\downarrow}\right) = \mathrm{r}_\beta^{n/2} \int_0^{2\pi} e^{in\phi} \mathrm{d}\hat{\mathfrak{m}}_{\omega_\infty}(\phi) = 0.$$

Therefore, if $\mathrm{r}_\beta > 0$, there is a unique probability measure allowing the $U(1)$–gauge symmetry of ω_∞: $\mathrm{d}\hat{\mathfrak{m}}_{\omega_\infty}(\phi)$ must be the uniform probability measure on $[0, 2\pi)$.

From Lemma 7.1 the cardinality of set of maximizers of (2.4) is at most 2. Indeed, away from any critical point, it is 1 whereas at a critical point it can be either 1 (second order phase transition) or 2 (first order phase transition). For more details, see Section 7. In both cases, we can use the same arguments as above. By similar estimates as in the proof of Lemma 6.6 it immediately follows that all limit points of the Gibbs states ω_N with parameters $(\beta_N, \gamma_N, \mu_N, \lambda_N, h_N)$ converging to $(\beta, \gamma, \mu, \lambda, h) \in \partial\mathcal{S}$ as $N \to \infty$, belongs to $\Omega_\beta = \Omega_\beta(\mu, \lambda, \gamma, h)$. Since the set of all $U(1)$–invariant equilibrium states from Ω_β is $\{\omega^{(\tau)}$ for any $\tau \in [0,1]\}$ with

$$\omega^{(\tau)}(\cdot) := (1-\tau)\,\omega_{\zeta_0}(\cdot) + \frac{\tau}{2\pi}\int_0^{2\pi} \omega_{\zeta_{\mathrm{c}_\beta}}(\cdot)\,\mathrm{d}\phi, \tag{6.57}$$

we obtain the second statement (ii). □

This theorem is a generalization of results obtained for the strong coupling[21] BCS model [7]. Note however, that Thirring's analysis [7] of the asymptotics of local Gibbs states comes from explicit computations, whereas we use the structure of sets of states, as explained for instance in [33].

Observe that Theorem 4.3 is a simple consequence of Theorem 6.15. Indeed, assume for instance that the order parameter $\mathrm{r}_\beta = \mathrm{r}_\beta(\mu, \lambda, \gamma, h)$ and the electron density per site $\mathrm{d}_\beta = \mathrm{d}_\beta(\mu, \lambda, \gamma, h)$ jumps respectively from $\mathrm{r}_\beta^- = 0$ to r_β^+ and from d_β^- to d_β^+ by crossing a critical chemical potential $\mu_\beta^{(c)}$ at fixed parameters $(\beta, \lambda, \gamma, h)$. An example of such behavior is given in figure 10 for an electron density smaller than one. If $\rho \in [\mathrm{d}_\beta^-, \mathrm{d}_\beta^+]$, then the unique solution $\mu_{N,\beta} = \mu_{N,\beta}(\rho, \lambda, \gamma, h)$ of (4.1) must converge towards $\mu_\beta^{(c)}$ as $N \to \infty$. Meanwhile, at fixed $(\beta, \mu_\beta^{(c)}, \lambda, \gamma, h)$

$$\omega_{\zeta_0}(n_\uparrow + n_\downarrow) = \mathrm{d}_\beta^- \text{ and } \omega_{\zeta_{\mathrm{c}_\beta^+}}(n_\uparrow + n_\downarrow) = \mathrm{d}_\beta^+,$$

with $\mathrm{c}_\beta^+ := \sqrt{\mathrm{r}_\beta^+}e^{i\phi}$ and $\phi \in [0, 2\pi)$. Any weak*–limit ω_∞ of local Gibbs states ω_N satisfies per construction

$$\omega_\infty(n_\uparrow + n_\downarrow) = \rho$$

and has the form $\omega^{(\tau)}(\cdot)$ (6.57), by Theorem 6.15. Hence, the Gibbs state ω_N converges in the weak*–topology towards $\omega^{(\tau_\rho)}(\cdot)$ with τ_ρ defined in Theorem 4.3. Indeed, the existence of the limits (i)–(iii) in Theorem 4.3 follows from the uniqueness of the limiting equilibrium state with fixed electron density $\rho \in [d_\beta^-, d_\beta^+]$.

We give now various important properties of densities in ground states, i.e., for $\beta = \infty$, which immediately follow from Theorem 6.14. Recall that the set Ω_∞ of ground states is the set of all weak* limit points as $n \to \infty$ of all equilibrium state sequences $\{\omega^{(n)}\}_{n\in\mathbb{N}}$ with diverging inverse temperature $\beta_n \to \infty$.

Take $\gamma > 0$ and parameters μ, λ, h such that $|\mu - \lambda| \neq \lambda + |h|$. Then the electron and Coulomb correlation densities equal respectively

$$\mathrm{d} := \omega(n_{\kappa(l),\uparrow} + n_{\kappa(l),\downarrow}) = \mathrm{d}_\infty \quad \text{and} \quad \mathrm{w} := \omega(n_{\kappa(l),\uparrow} n_{\kappa(l),\downarrow}) = \mathrm{w}_\infty, \tag{6.58}$$

for any ground state $\omega \in \Omega_\infty$ and $l \in \mathbb{N}$, cf. Corollaries 3.9 and 3.13.

If additionally $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$, we are in the superconducting phase for ground states, cf. Corollary 3.5. Indeed, for any $\varphi \in [0, 2\pi)$, there is a ground state $\omega \in \Omega_\infty$ such that for any $l \in \mathbb{N}$,

$$\omega(a_{\kappa(l),\downarrow} a_{\kappa(l),\uparrow}) = \mathrm{r}_{\max}^{1/2} e^{i\varphi}.$$

In the superconducting phase, from Corollary 3.13 we observe that $\mathrm{d}_\infty = 2\mathrm{w}_\infty$, whereas the magnetization density equals

$$\mathrm{m} := \omega(n_{\kappa(l),\uparrow} - n_{\kappa(l),\downarrow}) = \mathrm{m}_\infty = 0, \tag{6.59}$$

for any superconducting state $\omega \in \Omega_\infty$ and $l \in \mathbb{N}$. This is the Meißner effect, see Corollary 3.11. On the other hand, the Cauchy–Schwarz inequality for the states implies the inequalities

$$0 \leq \omega\left(n_{\kappa(l),\uparrow} n_{\kappa(l),\downarrow}\right) \leq \sqrt{\omega\left(n_{\kappa(l),\uparrow}\right)}\sqrt{\omega\left(n_{\kappa(l),\downarrow}\right)} \tag{6.60}$$

[21] See (1.2) with $\lambda = 0$ and $h = 0$.

for any $l \in \mathbb{N}$ and $\omega \in E_{\mathcal{U}}^{+}$. In fact, in the superconducting phase the second inequality of (6.60) is an equality for any $\omega \in \Omega_\infty$. Indeed, (6.59) and Corollary 3.13 yield

$$\omega(n_{\kappa(l),\uparrow} n_{\kappa(l),\downarrow}) = \omega(n_{\kappa(l),\uparrow}) = \omega(n_{\kappa(l),\downarrow}), \tag{6.61}$$

for any $\omega \in \Omega_\infty$ and $l \in \mathbb{N}$. It shows that 100% of electrons form Cooper pairs in superconducting ground states.

In the case where $h \neq 0$ with $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$ and $|\mu - \lambda| \neq \lambda + |h|$, the density vector $(\mathrm{d}, \mathrm{m}, \mathrm{w})$ defined by (6.58) and (6.59) is also unique as in the superconducting phase. It equals $(\mathrm{d}_\infty, \mathrm{m}_\infty, \mathrm{w}_\infty)$, see Corollaries 3.9, 3.11 and 3.13. However, if $h = 0$ with $\gamma < \Gamma_{|\mu-\lambda|,\lambda}$, or $\gamma = \Gamma_{|\mu-\lambda|,\lambda+|h|}$, or $|\mu - \lambda| = \lambda + |h|$, then the density vector $(\mathrm{d}, \mathrm{m}, \mathrm{w})$ belongs, in general, to a non trivial convex set. In other words, there are phase transitions involving to these densities. In particular, even in the case $h = 0$ where the Hamiltonian H_N (1.2) is spin invariant, there are ground states breaking the spin $SU(2)$–symmetry.

For instance, take $\beta, \gamma > 0$ and parameters μ, λ such that $|\mu - \lambda| < \lambda$ and $\gamma < \Gamma_{|\mu-\lambda|,\lambda}$. Then for any $\omega \in \Omega_\infty$ and $l \in \mathbb{N}$, the electron density equals $\mathrm{d} = \mathrm{d}_\infty = 1$, whereas the Coulomb correlation density is $\mathrm{w} = \mathrm{w}_\infty = 0$. In particular, the first inequality of (6.60) is an equality showing that 0% of electrons forms Cooper pairs. But, even if the magnetic field vanishes, i.e., $h = 0$, for any $x \in (-1, 1)$ there exists a ground state $\omega^{(x)} \in \Omega_\infty$ with magnetization density $\mathrm{m} = x$ (see (6.59) for the definition of m).

Therefore, all the thermodynamics of the strong coupling BCS–Hubbard model discussed in Sections 3.1–3.5 is encoded in the notion of equilibrium and ground states $\omega \in \Omega_\beta$ with $\beta \in (0, \infty]$. However, there is still an important open question related to the thermodynamics of this model. It concerns the problem of fluctuations of the Cooper pair condensate density (Theorem 3.1) or Cooper fields $\Phi_{\kappa(l)}$ and $\Psi_{\kappa(l)}$ (6.48) as a function of the temperature. Unfortunately, no result in that direction are known as soon as the thermodynamic limit is concerned. We prove however a simple statement about fluctuations of Cooper fields for pure states from Ω_β in the limit $\gamma\beta \to \infty$.

Theorem 6.16 (Fluctuations of Cooper fields)
Take $\beta, \gamma > 0$ and real numbers μ, λ, h away from any critical point. Then, for any pure state $\omega_{\zeta_{\mathrm{c}_\beta}} \in \Omega_\beta$ and $l \in \mathbb{N}$, the fluctuations of Cooper fields $\Phi_{\kappa(l)}$ and $\Psi_{\kappa(l)}$ (6.48) are bounded by

$$0 \leq \omega_{\zeta_{\mathrm{c}_\beta}} \left(\{\Phi_{\kappa(l)} - \omega_{\zeta_{\mathrm{c}_\beta}}(\Phi_{\kappa(l)})\}^2 \right) \leq 2\gamma^{-1}\beta^{-1},$$
$$0 \leq \omega_{\zeta_{\mathrm{c}_\beta}} \left(\{\Psi_{\kappa(l)} - \omega_{\zeta_{\mathrm{c}_\beta}}(\Psi_{\kappa(l)})\}^2 \right) \leq 2\gamma^{-1}\beta^{-1},$$

i.e., they vanish in the limit $\gamma\beta \to \infty$.

Proof: Recall that properties of pure states are characterized in Corollary 6.11, i.e., they are product states $\omega_{\zeta_{\mathrm{c}_\beta}}$ with the one–site state ζ_{c_β} being defined in (6.1). In particular, they satisfy (6.49). Now, to avoid triviality, assume that $\mathrm{c}_\beta := \mathrm{r}_\beta^{1/2} e^{i\phi} \neq 0$ and let $\mathfrak{f}(\tau)$ be the function defined for any $\tau \in \mathbb{R}$ by

$$\mathfrak{f}(\tau) := -\gamma |\mathrm{c}_\beta + \tau|^2 + p(\mathrm{c}_\beta + \tau).$$

Since $\mathrm{c}_\beta \neq 0$ is a maximizer of the function $-\gamma|c| + p(c)$ of $c \in \mathbb{C}$, one has $\partial_\tau^2 \mathfrak{f}(0) \leq 0$, i.e., $\partial_\tau^2 p(\mathrm{c}_\beta + \tau)|_{\tau=0} \leq 2\gamma$. From straightforward computations, observe that $p(\mathrm{c}_\beta + \tau)$ is a convex function of $\tau \in \mathbb{R}$ with

$$\beta^{-1}\gamma^{-2}\{\partial_\tau^2 p(\mathrm{c}_\beta + \tau)\}|_{\tau=0} = \omega_{\zeta_{\mathrm{c}_\beta}} \left(\{\Phi_{\kappa(l)} - \omega_{\zeta_{\mathrm{c}_\beta}}(\Phi_{\kappa(l)})\}^2 \right) \geq 0.$$

From this last equality combined with $\{\partial_\tau^2 p(\mathrm{c}_\beta + \tau)\}|_{\tau=0} \leq 2\gamma$, we deduce the theorem for $\Phi_{\kappa(l)}$. Moreover, from similar arguments using the function $\hat{\mathfrak{f}}(\tau) := \mathfrak{f}(i\tau)$ instead of $\mathfrak{f}$, the fluctuations of the Cooper field $\Psi_{\kappa(l)}$ are also bounded by $2\gamma^{-1}\beta^{-1}$. □

From Theorem 6.16, note that Cooper fields are c–numbers in the corresponding GNS–representation [32] of pure ground states defined as weak*–limits of pure equilibrium states:

Corollary 6.17 (Cooper fields for pure ground states)
Let $\omega \in \Omega_\infty$ be any weak–limit of pure equilibrium states and let $(\psi, \pi, \mathcal{H})$ be the corresponding GNS–representation of ω on bounded operators on the Hilbert space $\mathcal{H}$ with cyclic vacuum ψ. Then ω is pure and for any $l \in \mathbb{N}$, $\pi(\Phi_{\kappa(l)}) = \omega(\Phi_{\kappa(l)})\mathbb{I}_\mathcal{H}$ and $\pi(\Psi_{\kappa(l)}) = \omega(\Psi_{\kappa(l)})\mathbb{I}_\mathcal{H}$.*

Proof: A pure equilibrium state is a product state (6.7) and any weak*–limit of product states in $E_\mathcal{U}^{S,+}$ is also a product state. Thus, by Lemma 6.7, any ground state $\omega \in \Omega_\infty$ defined as the weak*–limit of pure equilibrium states is extremal in $E_\mathcal{U}^{S,+}$ and hence extremal in Ω_∞. Clearly, for such ground state, $\pi(\omega(\Phi_{\kappa(l)})) = \omega(\Phi_{\kappa(l)})\mathbb{I}_\mathcal{H}$ for any $l \in \mathbb{N}$. Let $\tilde{\Phi} := \Phi_{\kappa(l)} - \omega\left(\Phi_{\kappa(l)}\right)$. From Theorem 6.16 combined with the Cauchy–Schwarz inequality we obtain for any $A \in \mathcal{U}$ that

$$
\begin{aligned}
\left\|\pi(\tilde{\Phi})\pi(A)\psi\right\|_\mathcal{H}^2 &= \omega(A^*\tilde{\Phi}\tilde{\Phi}A) \leq \|A\|\sqrt{\omega\left(\tilde{\Phi}(\tilde{\Phi}AA^*\tilde{\Phi}^2)\right)} \\
&\leq \|A\|^2\|\tilde{\Phi}\|^{3/2}[\omega(\tilde{\Phi}^2)]^{1/4} = 0.
\end{aligned}
$$

From the cyclicity of ψ, it follows that $\pi(\Phi_{\kappa(l)}) = \omega(\Phi_{\kappa(l)})\mathbb{I}_\mathcal{H}$. The proof of $\pi(\Psi_{\kappa(l)}) = \omega(\Psi_{\kappa(l)})\mathbb{I}_\mathcal{H}$ is also performed in the same way. We omit the details. □

In particular, for such pure ground states ω in Ω_∞, correlation functions can explicitly be computed at any order in Cooper fields. For instance, for all $N \in \mathbb{N}$, all $k_j, l_j \in \mathbb{N}$, $m_j, n_j \in \mathbb{N}_0$, $j = 1, \ldots, N$, and any $A_n \in \mathcal{U}$, $n = 1, \ldots, N+1$, one has

$$
\begin{aligned}
&\omega\left(A_1\Phi_{\kappa(k_1)}^{m_1}\Psi_{\kappa(l_1)}^{n_1}A_2\ldots A_N\Phi_{\kappa(k_N)}^{m_N}\Psi_{\kappa(l_N)}^{n_N}A_{N+1}\right) \\
= \ &\omega(\Phi_{\kappa(k_1)}^{m_1})\omega(\Psi_{\kappa(l_1)}^{n_1})\ldots\omega(\Phi_{\kappa(k_N)}^{m_N})\omega(\Psi_{\kappa(l_N)}^{m_N})\,\omega\left(A_1\ldots A_{N+1}\right).
\end{aligned}
$$

7. Analysis of the variational problem

The variational problem (2.4) is quite explicit but for the reader convenience, we collect here some properties of its solution r_β w.r.t. $\beta, \gamma > 0$ and $\mu, \lambda, h \in \mathbb{R}$. We show in particular that $\mathrm{r}_\beta > 0$ exists in a non–empty domain of $(\beta, \gamma, \mu, \lambda, h)$ with some monotonicity properties as well as the existence of both first and second order phase transitions. We conclude this section by giving the asymptotics of r_β as $\beta \to \infty$, i.e., by proving Corollary 3.5.

1. We start by showing that $\mathrm{r}_\beta = 0$ for sufficiently small inverse temperatures β at fixed γ, μ, λ and h. Indeed, for any $r \geq 0$ one computes that

$$
\partial_r f\,(r) = \gamma\left(\frac{\gamma\sinh\left(\beta g_r\right)}{2g_r\left(e^{\lambda\beta}\cosh\left(\beta h\right) + \cosh\left(\beta g_r\right)\right)} - 1\right), \tag{7.1}
$$

cf. Theorem 2.1. Direct estimations show that if $0 < \beta < 2\gamma^{-1}$, then $\partial_r f(r) < 0$ for any $r \geq 0$, i.e., $\mathrm{r}_\beta = 0$.

2. Fix now $\beta > 0$ and $\mu, \lambda, h \in \mathbb{R}$, then $\mathrm{r}_\beta > 0$ for sufficiently large coupling constants γ. Indeed, for large enough $\gamma > 0$ there is, at least, one strictly positive solution $\tilde{\mathrm{r}}_\beta > 0$ of (2.5). Since direct computations using again (2.5) imply that

$$
\frac{d}{d\gamma}\left\{f\left(\beta, \mu, \lambda, \gamma, h; \tilde{\mathrm{r}}_\beta(\gamma)\right) - f\left(\beta, \mu, \lambda, \gamma, h; 0\right)\right\} = \tilde{\mathrm{r}}_\beta(\gamma) > 0,
$$

and

$$
f\left(\beta, \mu, \lambda, \gamma, h; \tilde{\mathrm{r}}_\beta\right) - f\left(\beta, \mu, \lambda, \gamma, h; 0\right) = \mathcal{O}\left(\gamma\right) \text{ as } \gamma \to \infty,
$$

for any fixed $\beta > 0$ and $\mu, \lambda, h \in \mathbb{R}$, there is a unique $\gamma_c > 2|\lambda - \mu|$ such that $f(\tilde{\mathrm{r}}_\beta) > f(0)$, i.e., $\mathrm{r}_\beta > 0$ for $\gamma > \gamma_c$. The domain of parameters $(\beta, \mu, \lambda, \gamma, h)$ where r_β is strictly positive is therefore non–empty, cf. figures 3–4.

3. To get an intuitive idea of the behavior of the function $f\,(r)$ (cf. Theorem 2.1), we analyze the cardinality of the set $\mathfrak{S}$ of strictly positive solutions of the gap equation (2.5):

Lemma 7.1 (Cardinality of the set $\mathfrak{S}$)
If $\beta\gamma \leq 6$, the gap equation (2.5) has at most one strictly positive solution, whereas it has, at most, two strictly positive solutions when $\beta\gamma > 6$.

Proof: From (7.1), any strictly positive maximizer $\mathrm{r}_\beta > 0$ of (2.4) is solution of the equation

$$\mathfrak{h}_1(g_r) = 0, \qquad \text{with} \quad \mathfrak{h}_1(x) := \frac{\gamma}{2x}\sinh(\beta x) - e^{\lambda\beta}\cosh(\beta h) - \cosh(\beta x). \tag{7.2}$$

This last equation is equivalent to the gap equation (2.5). For any $x > 0$, observe that

$$\partial_x \mathfrak{h}_1(x) = \frac{\beta\gamma}{2x}\cosh(x\beta) - \Big(\frac{\gamma}{2x^2} + \beta\Big)\sinh(x\beta) = 0 \tag{7.3}$$

if and only if

$$(2\beta^{-1}\gamma^{-1})^{1/2} y = \sqrt{\frac{y}{\tanh(y)} - 1} =: C(y), \quad y = \beta x > 0. \tag{7.4}$$

The map $y \mapsto C(y)$ is strictly concave for $y > 0$, $C(0) = 0$, and $\partial_y C(0) = (2/6)^{1/2}$. Therefore, if $\beta\gamma > 6$ there is a unique strictly positive solution $\widetilde{y} = \beta\widetilde{x} > 0$ of (7.4), and there is no strictly positive solution of (7.4) when $\beta\gamma < 6$. Since $\mathfrak{h}_1(0)$ could be negative in some cases and $\mathfrak{h}_1(x)$ diverges exponentially to $-\infty$ as $x \to \infty$, the cardinality of set of strictly positive solutions of the gap equation (2.5) is at most two if $\beta\gamma > 6$, or at most one if $\beta\gamma \leq 6$. $\square$

Consequently, if the gap equation (2.5) has no solution, then $f(r)$ is strictly decreasing for any $r \geq 0$. If the gap equation (2.5) has one unique solution $\mathrm{r}_\beta > 0$, the function $f(r)$ is increasing until its (strictly positive) maximizer $\mathrm{r}_\beta > 0$ and decreasing next for $r \geq \mathrm{r}_\beta$. Finally, when there are two strictly positive solutions of (2.5), the lower one must be one local minimum whereas the larger solution must be a local maximum. In this case the function $f(r)$ decreases for $r \geq 0$ until its local minimum, then increases until its local maximum, and finally decreases again to diverge towards $-\infty$. Note that none of these cases can be excluded, i.e., they all appear depending on $\beta, \gamma > 0$ and $\mu, \lambda, h \in \mathbb{R}$. See figures 3 and 18.

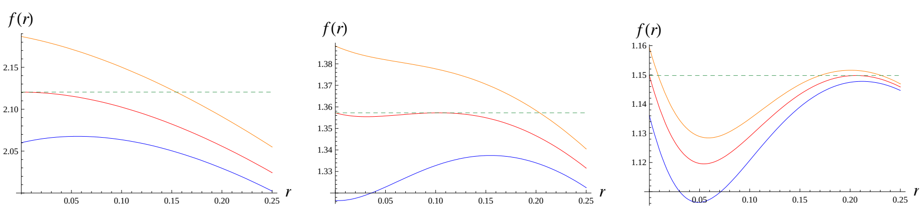

Figure 18: *Illustrations of the function $f(r)$ for $r \in [0, 1/4]$ at $(\mu, \gamma, h) = (1, 2.6, 0)$ with inverse temperatures $\beta = \beta_c - 0.3$ (orange line), $\beta = \beta_c$ (red line), $\beta = \beta_c + 0.5$ (blue line), and with coupling constants $\lambda = 0$ (left figure), $\lambda = 0.45$ (figure on the center) and $\lambda = 0.575$ (right figure). Here $\beta_c = \theta_c^{-1}$ is the critical inverse temperature which, from left to right, equals 2.04, 3.46 and 6.35 respectively.*

4. We study now the dependence of $\mathrm{r}_\beta > 0$ w.r.t. variations of each parameter. So, let us fix the parameters $\{\beta, \mu, \lambda, \gamma, h\} \backslash \{\nu\}$ with $\nu = \beta$, μ, λ, γ, or h and consider the function $\xi(r, \nu) := \partial_r f(r, \nu)$ for $r \geq 0$ and ν in the open set of definition of $f(r, \nu) = f(\beta, \mu, \lambda, \gamma, h; r)$, see (7.1). Recall that $\mathrm{r}_\beta > 0$ is a solution at $\nu = \nu_0$ of the gap equation (2.5), i.e., $\xi(\mathrm{r}_\beta, \nu_0) = 0$.

Straightforward computations imply that

$$\partial_r^2 f(r) = \frac{\gamma^4 \beta}{4 g_r^2 \left(e^{\lambda\beta}\cosh(\beta h) + \cosh(\beta g_r)\right)} \mathfrak{h}_2(g_r), \tag{7.5}$$

for any $r > 0$ with

$$\mathfrak{h}_2(x) := \frac{e^{\lambda\beta}\cosh(\beta h)\cosh(\beta x) + 1}{e^{\lambda\beta}\cosh(\beta h) + \cosh(\beta x)} - \frac{\sinh(\beta x)}{\beta x}. \tag{7.6}$$

It yields that there is at most one strictly positive solution, $\tilde{\mathrm{r}} \geq 0$ of $\partial_r \xi(r, \nu_0) = 0$ for each fixed set of parameters. For instance, if $e^{\lambda\beta}\cosh(\beta h) \leq 1$, then it is straightforward to check that $\partial_r \xi(r, \nu_0) < 0$ for any $r > 0$. In the situation where the gap equation (2.5) has two strictly positive solutions, $\mathrm{r}_\beta > 0$ cannot solve $\partial_r \xi(r, \nu_0) = 0$, since in this case the equation $\mathfrak{h}_2(x) = 0$ would have at least two strictly positive solutions, as r_β is a maximizer.

Consequently, to simplify our study we restrict on the very large set of parameters where $\partial_r \xi(\mathrm{r}_\beta, \nu_0) \neq 0$. In this case, the differential $d\xi$ has maximal rank at $(\mathrm{r}_\beta, \nu_0)$ and from the implicit function theorem, there are $\varepsilon > 0$ and a smooth and strictly positive function[22] $\mathrm{r}_\beta(\nu) > 0$ defined on the ball $B_\varepsilon(\nu_0)$ centered on the point ν_0 and with radius ε such that $\xi(\nu, \mathrm{r}_\beta(\nu)) = 0$ for any $\nu \in B_\epsilon(\nu_0)$. By continuity of the function $\partial_r \xi$ we can choose $\varepsilon > 0$ such that $\partial_r \xi(\nu, \mathrm{r}_\beta(\nu))$ does not change its sign for $\nu \in B_\epsilon(\nu_0)$. Thus $\mathrm{r}_\beta(\nu)$ describes the evolution of the solution of (2.4) for $\nu \in B_\epsilon(\nu_0)$. If $\mathrm{r}_\beta = \mathrm{r}_\beta(\nu_0) > 0$ is the unique maximizer of (2.4) with $\partial_r \xi(\mathrm{r}_\beta, \nu_0) \neq 0$, then the function $\mathrm{r}_\beta(\nu)$ describes the smooth evolution of the Cooper pair condensate density w.r.t. small perturbations of ν_0. Observe that

$$\partial_\nu \xi\left(\mathrm{r}_\beta\left(\nu\right), \nu\right) = \left\{\partial_\nu \mathrm{r}_\beta\left(\nu\right)\right\}\left\{\partial_r \xi\left(r, \nu\right)\right\}|_{r=\mathrm{r}_\beta(\nu)} + \left\{\partial_\nu \xi\left(r, \nu\right)\right\}|_{r=\mathrm{r}_\beta(\nu)} = 0$$

and $\left\{\partial_r \xi\left(r, \nu_0\right)\right\}|_{r=\mathrm{r}_\beta(\nu_0)} < 0$ because r_β is a maximizer. Consequently, one obtains

$$\mathrm{sgn}\left\{\partial_\nu \mathrm{r}_\beta\left(\nu_0\right)\right\} = \mathrm{sgn}\left\{\left\{\partial_\nu \partial_r f\left(r, \nu_0\right)\right\}|_{r=\mathrm{r}_\beta(\nu_0)}\right\}.$$

In other words, the function $\mathrm{r}_\beta(\nu)$ of $\nu \in B_\epsilon(\nu_0)$ is either increasing if

$$\left\{\partial_\nu \partial_r f\left(r, \nu_0\right)\right\}|_{r=\mathrm{r}_\beta(\nu_0)} > 0,$$

or decreasing if

$$\left\{\partial_\nu \partial_r f\left(r, \nu_0\right)\right\}|_{r=\mathrm{r}_\beta(\nu_0)} < 0,$$

as soon as $\mathrm{r}_\beta > 0$ is the unique maximizer of (2.4) with $\partial_r \xi(\mathrm{r}_\beta, \nu_0) \neq 0$.

5. By applying this last result respectively to $\nu_0 = \gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$ (Corollary 3.5) and $\nu_0 = h \in \mathbb{R}$, we obtain that $\mathrm{r}_\beta > 0$ is an increasing function of $\gamma > 0$ and a decreasing function of $|h|$ because via (2.5) one has

$$\left\{\partial_\gamma \partial_r f\left(r, \gamma\right)\right\}|_{r=\mathrm{r}_\beta} > 4\gamma^{-2}\left(\mu - \lambda\right)^2 \geq 0$$

at fixed parameters (β, μ, λ, h) and

$$\left\{\partial_h \partial_r f\left(r, h\right)\right\}|_{r=\mathrm{r}_\beta} = -\frac{2g_{\mathrm{r}_\beta}\beta e^{\lambda\beta}\sinh\left(\beta h\right)}{\sinh\left(\beta g_{\mathrm{r}_\beta}\right)}$$

at fixed $(\beta, \mu, \lambda, \gamma)$.

6. If $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$, for any fixed $(\beta, \gamma, \lambda, h)$ the order parameter $\mathrm{r}_\beta > 0$ is a decreasing function of $|\mu - \lambda|$ under the condition that $e^{\lambda\beta}\cosh\left(\beta h\right) \leq 1$, as

$$\left\{\partial_\mu \partial_r f\left(r, \mu\right)\right\}|_{r=\mathrm{r}_\beta} = \frac{\gamma^2\beta\left(\mu - \lambda\right)}{2g_r^2\left(e^{\lambda\beta}\cosh\left(\beta h\right) + \cosh\left(\beta g_{\mathrm{r}_\beta}\right)\right)}\mathfrak{h}_2\left(g_{\mathrm{r}_\beta}\right),$$

cf. (7.6). If $e^{\lambda\beta}\cosh\left(\beta h\right) > 1$, the behavior of $\mathrm{r}_\beta > 0$ is not anymore monotone as a function of $|\mu - \lambda|$ (λ being fixed), cf. figure 10.

The behavior of r_β as a function of λ or β is also not clear in general. But, at least as a function of the inverse temperature $\beta > 0$, we can give simple sufficient conditions to get its monotonicity. Indeed, direct computations show that

$$\begin{aligned}\left\{\partial_\beta \partial_r f\left(r, \beta\right)\right\}|_{r=\mathrm{r}_\beta} &= \left(\gamma + 2\lambda\right)g_{\mathrm{r}_\beta}\frac{\cosh\left(\beta g_{\mathrm{r}_\beta}\right)}{\sinh\left(\beta g_{\mathrm{r}_\beta}\right)} - \left(\lambda\gamma + 2g_{\mathrm{r}_\beta}^2\right) \\ &\quad -2hg_{\mathrm{r}_\beta}\frac{e^{\lambda\beta}\sinh\left(\beta h\right)}{\sinh\left(\beta g_{\mathrm{r}_\beta}\right)}.\end{aligned}$$

[22] If $\nu = \beta$, then of course $\mathrm{r}_\beta(\nu) := \mathrm{r}_\nu$.

By combining this last equality with (2.5), we then get that

$$\{\partial_\beta \partial_r f(r,\beta)\}|_{r=\mathrm{r}_\beta} \geq 0 \tag{7.7}$$

with $\mathrm{r}_\beta > 0$ if and only if

$$g_{\mathrm{r}_\beta}^2 \leq \frac{\gamma\left(\gamma\cosh\left(\beta g_{\mathrm{r}_\beta}\right) - 2e^{\lambda\beta}\cosh\left(\beta h\right)\left(\lambda + h\tanh\left(\beta h\right)\right)\right)}{4\left(\cosh\left(\beta g_{\mathrm{r}_\beta}\right) + e^{\lambda\beta}\cosh\left(\beta h\right)\right)}. \tag{7.8}$$

From (2.5) combined with $\tanh(x) < 1$, we also have

$$g_{\mathrm{r}_\beta}^2 < \frac{\gamma^2\cosh^2\left(\beta g_{\mathrm{r}_\beta}\right)}{4\left(\cosh\left(\beta g_{\mathrm{r}_\beta}\right) + e^{\lambda\beta}\cosh\left(\beta h\right)\right)^2}. \tag{7.9}$$

Therefore, a sufficient condition to satisfy the inequality (7.8) is obtained by bounding the r.h.s. of (7.9) with the r.h.s. of (7.8). From (2.5) this implies the condition

$$g_{\mathrm{r}_\beta} \geq \left(\lambda + h\tanh\left(\beta h\right)\right)\tanh\left(\beta g_{\mathrm{r}_\beta}\right),$$

under which r_β is an increasing function of $\beta > 0$. This inequality is also equivalent to

$$g_{\mathrm{r}_\beta} \leq \tanh\left(\beta g_{\mathrm{r}_\beta}\right)\left(\frac{\gamma}{2} - \frac{e^{\lambda\beta}\cosh\left(\beta h\right)}{\cosh\left(\beta g_{\mathrm{r}_\beta}\right)}\left(\lambda + h\tanh\left(\beta h\right)\right)\right).$$

In particular, by using again the gap equation (2.5), if

$$\gamma > 2\left(\lambda + h\tanh\left(\beta h\right)\right)\left(1 + \frac{e^{\lambda\beta}\cosh\left(\beta h\right)}{\cosh\left(\beta g_{\mathrm{r}_\beta}\right)}\right),$$

then $\mathrm{r}_\beta > 0$ is an increasing function of $\beta > 0$. Since $\tanh x \leq 1$, another sufficient condition to get (7.7) is $\lambda + |h| \leq g_{\mathrm{r}_\beta}$. In particular, if $\lambda < |\mu - \lambda|$ and $\gamma > \Gamma_{|\mu-\lambda|,\lambda+|h|}$ with h sufficiently small, then $\mathrm{r}_\beta > 0$ is again an increasing function of $\beta > 0$.

Therefore, the domain of $(\mu, \lambda, \gamma, h)$ where $\mathrm{r}_\beta > 0$ is proven to be an increasing function of $\beta > 0$ is rather large. Actually, from a huge number of numerical computations, we conjecture that $\mathrm{r}_\beta > 0$ is always an increasing function of $\beta > 0$. In other words, this conjecture implies that the condition expressed in Corollary 3.5 on $(\mu, \lambda, \gamma, h)$ should be necessary to obtain a superconductor at a fixed temperature.

7. Observe that the order of the phase transition depends on the parameters. For instance, assume $\lambda \leq 0$, $h = 0$ and $\gamma > \Gamma_{|\mu-\lambda|,\lambda}$. Then, at any inverse temperature $\beta > 0$ it follows from (7.5) that $f(r)$ is a strictly concave function of $r > 0$. This property justifies the existence and uniqueness of the inverse temperature β_c solution of the equation

$$\frac{\tanh\left(\beta|\mu-\lambda|\right)}{|\mu-\lambda|} = \frac{2}{\gamma}\left(1 + \frac{e^{\lambda\beta}}{\cosh\left(\beta|\mu-\lambda|\right)}\right),$$

i.e., (2.5) for $\lambda \leq 0$, $h = 0$ and $r = 0$. In particular, β_c is such that the Cooper pair condensate density continuously goes from $\mathrm{r}_\beta = 0$ for $\beta \leq \beta_c$ to $\mathrm{r}_\beta > 0$ for $\beta > \beta_c$. In this case the superconducting phase transition is of second order, cf. figure 3.

The appearance of a first order phase transition at some fixed $(\mu, \lambda, \gamma, h)$ is also not surprising. Indeed, recall that the function $f(r)$ may have a local minimum and a local maximum, see discussions below Lemma 7.1. For instance, assume now $\lambda = \mu > 0$, $h = 0$ and $4\lambda = \Gamma_{0,\lambda} < \gamma \leq 6\lambda$. Then, from (7.1) for $r = 0$,

$$\partial_r f\left(0\right) = \frac{\gamma}{e^{\lambda\beta} + 1}\left(\frac{\gamma\beta}{2} - \left(e^{\lambda\beta} + 1\right)\right).$$

Since by explicit computations

$$\min_{x>0}\left\{\frac{e^x + 1}{x}\right\} > 3,$$

it follows that $\partial_r f(0) < 0$ for any $\beta > 0$ whenever $\lambda = \mu > 0$, $h = 0$ and $0 < \gamma \leq 6\lambda$. Therefore, as soon as there is a superconducting phase transition, for instance if $4\lambda < \gamma \leq 6\lambda$ (cf. Corollary 3.5), the function r_β of $\beta > 0$ must be discontinuous at the critical point. This case is an example of a first order superconducting phase transition. Numerical illustrations of a similar first order phase transition are also given in figure 3.

8. We conclude this section by a computation of the asymptotics of the order parameter r_β as $\beta \rightarrow \infty$. We prove in particular Corollary 3.5.

From (2.6), we already know that $\mathrm{r}_\beta = 0$ for any $\gamma \leq 2|\tilde{\mu}_\lambda|$ with $\tilde{\mu}_\lambda := \mu - \lambda$. Therefore, we consider here that $\gamma > 2|\tilde{\mu}_\lambda|$ and we look for the domain where the parameter r_β is strictly positive in the limit $\beta \rightarrow \infty$. Recall that r_β is solution of the variational problem (2.4), i.e.,

$$\frac{1}{\beta}\ln 2 + \sup_{r\geq 0} f(r) = -\gamma \mathrm{r}_\beta + \frac{1}{\beta}\ln\left\{e^{\beta h} + e^{-\beta h} + e^{\beta\left(g_{\mathrm{r}_\beta} - \lambda\right)} + e^{-\beta\left(g_{\mathrm{r}_\beta} + \lambda\right)}\right\}. \tag{7.10}$$

When $\beta \rightarrow \infty$ the last exponential term can always be neglected for our analysis since $g_{\mathrm{r}_\beta} \geq 0$.

Now, assume first that $g_0 = |\tilde{\mu}_\lambda| > \lambda + |h|$. Then $g_r > \lambda + |h|$ for any $r \geq 0$ and when $\beta \rightarrow \infty$ the function $f(r)$ converges to

$$w(r) := -\gamma r + g_r - \lambda.$$

In particular, the order parameter r_β converges towards the unique maximizer $\mathrm{r}_{\max}$ (2.6) of the function $w(r)$ for $r \geq 0$, i.e.,

$$\mathrm{r}_\infty := \lim_{\beta\rightarrow\infty} \mathrm{r}_\beta = \mathrm{r}_{\max}, \tag{7.11}$$

for any $\gamma > 2|\tilde{\mu}_\lambda|$ and real numbers μ, λ, h satisfying $|\tilde{\mu}_\lambda| > \lambda + |h|$.

Assume now that $|\tilde{\mu}_\lambda| \leq \lambda + |h|$ and let $\mathrm{r}_{\min}$ be the solution of $g_r = \lambda + |h|$, i.e.,

$$\mathrm{r}_{\min} := \gamma^{-2}\left((\lambda + |h|)^2 - \tilde{\mu}_\lambda^2\right) \geq 0. \tag{7.12}$$

Then, for any $r \in [0, \mathrm{r}_{\min}]$

$$f(r) = -\gamma r + |h| + o(1) \text{ as } \beta \rightarrow \infty.$$

In particular, since $\gamma > 0$,

$$\sup_{0\leq r\leq \mathrm{r}_{\min}} f(r) = f(\delta) = |h| + o(1), \quad \text{with } \delta = o(1) \text{ as } \beta \rightarrow \infty. \tag{7.13}$$

The solution r_β of the variational problem (7.10) converges either to 0, or to some strictly positive value $\mathrm{r}_\infty > \mathrm{r}_{\min}$. In the case where $\mathrm{r}_\infty > \mathrm{r}_{\min}$, we would have

$$f(\mathrm{r}_\infty) = w(\mathrm{r}_\infty) + o(1) \text{ as } \beta \rightarrow \infty. \tag{7.14}$$

Now, if $|\tilde{\mu}_\lambda| \leq \lambda + |h|$ and $\gamma \leq 2(\lambda + |h|)$, then $\mathrm{r}_{\min} \geq \mathrm{r}_{\max}$, cf. (2.6) and (7.12). In this regime, straightforward computations show that

$$|h| - \sup_{r\geq \mathrm{r}_{\min}} w(r) = |h| - w(\mathrm{r}_{\min}) = \gamma^{-1}\left((|h| + \lambda)^2 - \tilde{\mu}_\lambda^2\right) \geq 0. \tag{7.15}$$

In other words, the order parameter r_β converges towards

$$\mathrm{r}_\infty := \lim_{\beta\rightarrow\infty} \mathrm{r}_\beta = 0, \tag{7.16}$$

for any $\gamma \leq 2(\lambda + |h|)$ and real numbers μ, λ, h satisfying $|\tilde{\mu}_\lambda| \leq \lambda + |h|$.

However, if $|\tilde{\mu}_\lambda| \leq \lambda + |h|$ and $\gamma > 2(\lambda + |h|)$, then $\mathrm{r}_{\min} < \mathrm{r}_{\max}$. In particular one gets

$$|h| - \sup_{r\geq \mathrm{r}_{\min}} w(r) = |h| - w(\mathrm{r}_{\max}) = -\frac{1}{4\gamma}\left(\gamma - \tilde{\Gamma}_{|\tilde{\mu}_\lambda|,\lambda+|h|}\right)\left(\gamma - \Gamma_{|\tilde{\mu}_\lambda|,\lambda+|h|}\right), \tag{7.17}$$

with $\Gamma_{x,y} \geq 2y$ defined for any $x \in \mathbb{R}_+$ and $y \in \mathbb{R}$ in Corollary 3.5 and

$$\tilde{\Gamma}_{|\tilde{\mu}_\lambda|,\lambda+|h|} := 2\left(\lambda + |h| - \sqrt{(\lambda+|h|)^2 - \tilde{\mu}_\lambda^2}\right) \leq 2\,|\tilde{\mu}_\lambda|\,.$$

In particular,

$$\sup_{r\geq \mathrm{r}_{\min}} w\,(r) = w\,(\mathrm{r}_{\max}) > |h|\,, \tag{7.18}$$

for any $\gamma > \Gamma_{|\tilde{\mu}_\lambda|,\lambda+|h|} \geq 2|\tilde{\mu}_\lambda|$. Therefore, by combining (7.13) with (7.14) and (7.18), we obtain

$$\mathrm{r}_\infty := \lim_{\beta\to\infty} \mathrm{r}_\beta = \mathrm{r}_{\max}, \tag{7.19}$$

for any $\gamma > \Gamma_{|\tilde{\mu}_\lambda|,\lambda+|h|}$ and real numbers μ, λ, h satisfying $|\tilde{\mu}_\lambda| \leq \lambda + |h|$.

Finally, if $\gamma = \Gamma_{|\tilde{\mu}_\lambda|,\lambda+|h|}$ and $|\tilde{\mu}_\lambda| < \lambda+|h|$, observe that (7.17) is zero. So, we analyze the next order term to know which number, 0 or $\mathrm{r}_{\max}$, maximizes the function $f\,(r)$ when $\beta \to \infty$. On the one hand, straightforward estimations imply that

$$f\,(0) - |h| = \beta^{-1}\left(e^{-\beta(\lambda+|h|-|\tilde{\mu}_\lambda|)} + e^{-2\beta|h|}\right)(1 + o\,(1)) \text{ as } \beta \to \infty. \tag{7.20}$$

On the other hand, if $\gamma = \Gamma_{|\tilde{\mu}_\lambda|,\lambda+|h|}$ with $|\tilde{\mu}_\lambda| < \lambda + |h|$, then by using (2.6) one obtains

$$f\,(\mathrm{r}_{\max}) - |h| = \beta^{-1} e^{-\beta\sqrt{(\lambda+|h|)^2-\tilde{\mu}_\lambda^2}}\,(1 + o\,(1)) \text{ as } \beta \to \infty. \tag{7.21}$$

Therefore, if $\gamma = \Gamma_{|\tilde{\mu}_\lambda|,\lambda+|h|}$ and $|\tilde{\mu}_\lambda| < \lambda+|h|$, it is trivial to check from (7.20)-(7.21) that $f(0) > f(\mathrm{r}_{\max})$ when $\beta \to \infty$.

Consequently, the limits (7.11), (7.16) and (7.19) together with (2.6) imply Corollary 3.5 for any $\gamma \neq \Gamma_{|\mu-\lambda|,\lambda+|h|}$, whereas if $\gamma = \Gamma_{|\mu-\lambda|,\lambda+|h|}$, the order parameter r_β converges to $\mathrm{r}_\infty = 0$.

8. Appendix: Griffiths arguments

As we have an explicit representation of the pressure, it can be verified in some cases that r_β is a C^1–function[23] of parameters implying that $\mathrm{p}\,(\beta,\mu,\lambda,\gamma,h)$ is differentiable w.r.t. parameters. In this particular situation, the proofs of Theorems 3.1, 3.3, 3.8, 3.10, 3.12 and 3.14 done in Section 6.2 could also be performed without our notion of equilibrium states by using Griffiths arguments [29, 30, 31], which are based on convexity properties of the pressure. We explain it shortly and we conclude by a discussion of an alternative proof of Theorem 3.3.

Remark 8.1 *Our method gives access to all correlation functions at once (cf. Theorem 6.15). It is generalized in [18] to all translation invariant Fermi systems. However, computing all correlation functions with Griffiths arguments [29, 30, 31] requires the differentiability of the pressure w.r.t. any perturbation as well as the computation of its corresponding derivative. This is generally a very hard task, for instance for correlation functions involving many lattice points.*

1. Take self–adjoint operators $\mathfrak{P}_N$ acting on the fermionic Fock space and assume the existence of the (infinite volume) grand–canonical pressure

$$\mathrm{p}_\varepsilon\,(\beta,\mu,\lambda,\gamma,h) := \lim_{N\to\infty} \mathrm{p}_{N,\varepsilon}\,(\beta,\mu,\lambda,\gamma,h)$$

for any fixed ε in a neighborhood $\mathcal{V}$ of 0. In this case, observe that the finite volume pressure

$$\mathrm{p}_{N,\varepsilon}\,(\beta,\mu,\lambda,\gamma,h) := \frac{1}{\beta N} \ln \mathrm{Trace}\left(e^{-\beta(\mathrm{H}_N - \varepsilon\mathfrak{P}_N)}\right)$$

is convex as a function of $\varepsilon \in \mathcal{V}$ and

$$\partial_\varepsilon \mathrm{p}_{N,0} = N^{-1}\omega_N\,(\mathfrak{P}_N)\,.$$

[23]For instance, for special choices of parameters one could check that $\partial_r \xi(\mathrm{r}_\beta, \nu_0) \neq 0$, see Section 7.

Consequently, the point-wise convergence of the function $\mathrm{p}_{N,\varepsilon}$ towards p_{ε} implies that

$$\liminf_{N\to\infty}\left\{\lim_{\varepsilon\to 0^-}\partial_\varepsilon \mathrm{p}_{N,\varepsilon}\right\}\geq \lim_{\varepsilon\to 0^-}\partial_\varepsilon \mathrm{p}_{\varepsilon} \text{ and } \limsup_{N\to\infty}\left\{\lim_{\varepsilon\to 0^+}\partial_\varepsilon \mathrm{p}_{N,\varepsilon}\right\}\leq \lim_{\varepsilon\to 0^+}\partial_\varepsilon \mathrm{p}_{\varepsilon}, \tag{8.1}$$

see Griffiths lemma [30, 31] or [29, Appendix C]. In particular, one gets

$$\lim_{N\to\infty}\{\partial_\varepsilon \mathrm{p}_{N,0}\} = \lim_{N\to\infty}\left\{N^{-1}\omega_N\left(\mathfrak{P}_N\right)\right\} = \partial_\varepsilon \mathrm{p}_{\varepsilon=0}, \tag{8.2}$$

under the assumption that p_ε is differentiable at $\varepsilon = 0$.

2. Therefore, by taking

$$\mathfrak{P}_N = \sum_{x,y\in\Lambda_N} a^*_{x,\uparrow}a^*_{x,\downarrow}a_{y,\downarrow}a_{y,\uparrow},$$

we obtain from (8.2) that

$$\lim_{N\to\infty}\left\{\frac{1}{N^2}\sum_{x,y\in\Lambda_N} a^*_{x,\uparrow}a^*_{x,\downarrow}a_{y,\downarrow}a_{y,\uparrow}\right\} = \partial_\gamma \mathrm{p}\left(\beta,\mu,\lambda,\gamma,h\right),$$

as soon as the (infinite volume) pressure $\mathrm{p}\left(\beta,\mu,\lambda,\gamma,h\right)$ has continuous derivative w.r.t. $\gamma > 0$. Combined with Theorem 2.1 and (2.5) we would obtain Theorem 3.1. Meanwhile, Theorem 3.8, 3.10, 3.12 and 3.14 could have been deduced in the same way from (8.2) combined with explicit computations using (2.5).

3. A direct proof of Theorem 3.3 using Griffiths arguments is more delicate. One uses similar arguments as in [29, 42]. We give them for the interested reader.

For any $\phi \in [0, 2\pi)$, first recall that the pressure $\mathrm{p}_{\alpha,\phi}$ associated with $\mathrm{H}_{N,\alpha,\phi}$ (3.1) in the thermodynamic limit is given by (6.41), which equals (6.43). Additionally, if the parameters β, μ, λ, γ, and h are such that (2.4) has a unique maximizer r_β, then the variational problem (6.43) has a unique maximizer $\mathrm{c}_{\beta,\alpha,\phi} \in e^{i\phi}\mathbb{R}$ for $\alpha > 0$ sufficiently small, and $\mathrm{c}_{\beta,\alpha,\phi}$ converges to $\mathrm{r}_\beta^{1/2}e^{i\phi}$ as $\alpha \to 0$, see proof of Theorem 6.12.

Now, let us denote by

$$\mathfrak{N}_N := \sum_{x\in\Lambda_N}\left(n_{x,\uparrow}+n_{x,\downarrow}\right)$$

the full particle number operator. By straightforward computations observe that

$$[a_{x,\uparrow}, \mathfrak{N}_N] = a_{x,\uparrow} \text{ and } [a_{x,\downarrow}, \mathfrak{N}_N] = a_{x,\downarrow}, \tag{8.3}$$

for any lattice site labelled by $x \in \Lambda_N$, where $[A, B] := AB - BA$. Therefore the unitary operator $U_\phi := e^{-\frac{i\phi}{2}\mathfrak{N}_N}$ realizes a global gauge transformation because one deduces from (8.3) that

$$U_\phi a_{x,\uparrow}U^*_\phi = e^{\frac{i\phi}{2}}a_{x,\uparrow} \quad\text{and}\quad U_\phi a_{x,\downarrow}U^*_\phi = e^{\frac{i\phi}{2}}a_{x,\downarrow}. \tag{8.4}$$

In particular the unitary transformation of the Hamiltonian $\mathrm{H}_{N,\alpha,\phi}$ (3.1) equals

$$U_\phi \mathrm{H}_{N,\alpha,\phi}U^*_\phi = \mathrm{H}_{N,\alpha,0}.$$

It implies on the corresponding Gibbs states (6.42) that

$$\omega_{N,\alpha,\phi}\left(\mathfrak{B}_N\right) = e^{i\phi}\omega_{N,\alpha,0}\left(\mathfrak{B}_N\right), \tag{8.5}$$

with the operator $\mathfrak{B}_N$ be defined by

$$\mathfrak{B}_N := \sum_{x\in\Lambda_N} a_{x,\downarrow}a_{x,\uparrow}.$$

In other words, it suffices to prove Theorem 3.3 for $\phi = 0$.

Take $\phi = 0$. Observe that

$$0 = \omega_{N,\alpha,0}\left([\mathrm{H}_{N,\alpha,0}, \mathfrak{N}_N]\right) = \alpha\omega_{N,\alpha,0}\left(\mathfrak{B}_N - \mathfrak{B}_N^*\right). \tag{8.6}$$

Additionally, by using the positive semidefinite Bogoliubov–Duhamel scalar product

$$(X,Y)_{\mathrm{H}_{N,\alpha,0}} := \beta^{-1} e^{-\beta N \mathrm{p}_{N,\alpha,0}(\beta,\mu,\lambda,\gamma,h)} \int_0^\beta \mathrm{Trace}\left(e^{-(\beta-\tau)\mathrm{H}_{N,\alpha,0}} X^* e^{-\tau \mathrm{H}_{N,\alpha,0}} Y\right) \mathrm{d}\tau$$

w.r.t. the Hamiltonian $\mathrm{H}_{N,\alpha,0}$ (see, e.g., [25, 29, 42]), one gets that

$$\begin{aligned} 0 &\leq \beta\left([\mathfrak{N}_N, \mathrm{H}_{N,\alpha,0}], [\mathfrak{N}_N, \mathrm{H}_{N,\alpha,0}]\right)_{\mathrm{H}_{N,\alpha,0}} \\ &= \omega_{N,\alpha,0}\left([\mathfrak{N}_N, [\mathrm{H}_{N,\alpha,0}, \mathfrak{N}_N]]\right) = \alpha\omega_{N,\alpha,0}\left(\mathfrak{B}_N + \mathfrak{B}_N^*\right). \end{aligned} \tag{8.7}$$

So, by combining (8.6) with (8.7) it follows that

$$\omega_{N,\alpha,0}\left(\mathfrak{B}_N\right) = \omega_{N,\alpha,0}\left(\mathfrak{B}_N^*\right) \geq 0$$

for any $\alpha \geq 0$. In particular $\omega_{N,\alpha,0}\left(\mathfrak{B}_N\right) = \omega_{N,\alpha,0}\left(\mathfrak{B}_N^*\right)$ is a real number.

The function $\mathrm{p}_{N,\alpha,0}$ is a convex function of $\alpha \geq 0$ because

$$\begin{aligned} &\beta\Big(\left\{(\mathfrak{B}_N + \mathfrak{B}_N^*) - \omega_{N,\alpha,0}\left(\mathfrak{B}_N + \mathfrak{B}_N^*\right)\right\}, \left\{(\mathfrak{B}_N + \mathfrak{B}_N^*) - \omega_{N,\alpha,0}\left(\mathfrak{B}_N + \mathfrak{B}_N^*\right)\right\} \Big)_{\mathrm{H}_{N,\alpha,0}} \\ = \; & \partial_\alpha^2 \mathrm{p}_{N,\alpha,0}\left(\beta,\mu,\lambda,\gamma,h\right). \end{aligned}$$

Then, under the assumption that $\mathrm{p}_{\alpha,0}$ is differentiable at $\alpha = 0$ away from any critical point, the equations (8.2), with

$$\mathfrak{P}_N = \mathfrak{B}_N + \mathfrak{B}_N^*$$

and (6.43), imply that

$$\begin{aligned} \lim_{N\to\infty}\left(\frac{1}{N}\omega_{N,\alpha,0}\left(\mathfrak{B}_N + \mathfrak{B}_N^*\right)\right) &= \lim_{N\to\infty}\partial_\alpha\left(\frac{1}{\beta N}\ln \mathrm{Trace}\left(e^{-\beta \mathrm{H}_{N,\alpha,0}}\right)\right) \\ &= \partial_\alpha \mathrm{p}_{\alpha,0}\left(\beta,\mu,\lambda,\gamma,h\right) \\ &= \zeta_{\mathrm{c}_{\beta,\alpha,0}}\left(a_\downarrow^* a_\uparrow^* + a_\uparrow a_\downarrow\right), \end{aligned}$$

for any $\alpha > 0$ sufficiently small and with $\zeta_c(\cdot)$ defined for any $c \in \mathbb{C}$ by (6.1).

Returning back to the original Hamiltonian $\mathrm{H}_{N,\alpha,\phi}$ (3.1) for any $\phi \in [0, 2\pi)$, we conclude from (8.5) combined with the last equalities that

$$\lim_{N\to\infty}\left\{\frac{1}{N}\sum_{x\in\Lambda_N}\omega_{N,\alpha,\phi}\left(a_{x,\uparrow}a_{x,\downarrow}\right)\right\} = \frac{e^{i\phi}}{2}\zeta_{\mathrm{c}_{\beta,\alpha,0}}\left(a_\downarrow^* a_\uparrow^* + a_\uparrow a_\downarrow\right).$$

Therefore, by taking the limit $\alpha \to 0$, Theorem 3.3 would follow if one additionally checks that $\mathrm{p}_{\alpha,0}$ is differentiable at $\alpha = 0$ away from any critical point.

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