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The Stability of the Peierls Instability for Ring-Shaped Molecules

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Abstract
We investigate the conventional tight-binding model of L π-electrons on a ring-shaped molecule of L atoms with nearest neighbor hopping. The hopping amplitudes, $t(w)$, depend on the atomic spacings, w, with an associated distortion energy $V(w)$. A Hubbard type on-site interaction as well as nearest-neighbor repulsive potentials can also be included. We prove that when $L = 4k+2$ the minimum energy E occurs either for equal spacing or for alternating spacings (dimerization); nothing more chaotic can occur. In particular this statement is true for the Peierls-Hubbard Hamiltonian which is the case of linear $t(w)$ and quadratic $V(w)$, i.e., $t(w) = t_0 - \alpha w$ and $V(w) = k(w-a)^2$, but our results hold for any choice of couplings or functions $t(w)$ and $V(w)$. When $L = 4k$ we prove that more chaotic minima *can* occur, as we show in an explicit example, but the alternating state is always asymptotically exact in the limit $L \to \infty$. Our analysis suggests three interesting conjectures about how dimerization stabilizes for large systems. We also treat the spin-Peierls problem and prove that nothing more chaotic than dimerization occurs for $L = 4k+2$ *and* $L = 4k$.

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1. INTRODUCTION

To derive the shape (and other properties) of molecules from first principles has been an actively pursued goal since the early days of quantum mechanics. Many of the insights into the structure of molecules like benzene and its relatives have, however, been obtained using drastically simplified models. The Schrödinger equation for all the nuclei and electrons in such a molecule involves many dozens or even hundreds of degrees of freedom and, therefore, simpler models with a reduced number of degrees of freedom are a necessity. In the case of benzene the introduction of the Hückel model [**1**] played an important role. This model is standard textbook material for organic chemistry students (see e.g. [**2**]). London [**3**] used the Hückel model to explain the large diamagnetic anisotropy of aromatic compounds and certain other materials quite successfully. A similar approach was used earlier by Jones in his work on bismuth and bismuth alloys [**4**].

In this paper we are interested in ring-shaped molecules of the type $(CH)_L$, for *even* L, the so-called *annulenes* (sometimes called cyclic polyenes). The Hückel model for $[L]$-annulene describes the L $\pi-$electrons (one for each carbon atom) as hopping from one carbon atom to the next (tight-binding approximation). The carbon atoms are located at the L sites of a ring-shaped geometry, so $L+1 \equiv 1$. The Coulomb interaction between the electrons is ignored in the Hückel model but we will include the Hubbard [**5**] on-site interaction as in the work of Pariser-Parr [**6**] and Pople [**7**], in our study (a nearest neighbour repulsion can also be included).

$$H = -\sum_{j=1}^{L} \sum_{\sigma=\uparrow,\downarrow} t_j c^\dagger_{j+1,\sigma} c_{j\sigma} + \text{ h.c. } + U \sum_{j=1}^{L} (n_{j\uparrow} - \tfrac{1}{2})(n_{j\downarrow} - \tfrac{1}{2}) \quad . \tag{1.1}$$

Here $c^\dagger_{j+1,\sigma}$ and $c_{j\sigma}$ are the usual fermion creation and annihilation operators for a particle of spin σ at site j. The number operators are $n_{j\sigma} = c^\dagger_{j\sigma} c_{j\sigma}$. The hopping matrix elements are real, but they can be multiplied by complex phases if a magnetic field is present. (In (1.1) we write $(n_{j\sigma} - \frac{1}{2})$ instead of the customary $n_{j\sigma}$; the difference amounts only to the addition of trivial terms in the Hamiltonian, but these are convenient because they ensure — via hole-particle symmetry — that the expected particle number in the grand canonical ensemble is $\langle N \rangle = L$, i.e., the "half-filled band".) The real parameter U represents the strength of the on-site interaction of two particles and the Hückel approximation consists in setting $U = 0$. The set of t_j's will be denoted by $\{t_j\}$. The dependence of the Hamiltonian on the parameters will be made explicit, where needed, with a notation of the type $H(\{t_j\}), H(\{t_j\}, U)$ etc.. For a review of rigorous results on the Hubbard model see [**8**].

The hopping matrix element t_j is a resonance integral between orbitals at the sites j and $j+1$ and therefore depends on the real space distance w_j between these sites. A typical choice is $t_j = t_0 - \alpha w_j$ [**9**]. A more realistic choice would be $t_j = t_0 \exp(-\alpha w_j)$ or some other rapidly decaying function of w_j. If one adds to the Hubbard Hamiltonian (even in the Hückel approximation) a term describing the interaction between the carbon ions (the energy of lattice distortions) one obtains a model that, in spite of its extreme simplicity, serves very well to explain a number of phenomena in annulenes and linear $(CH)_x$ (polyacetylene) [**10**].

For a recent review see the references [**11,12**]. Although in more refined models the lattice distortions should be treated as quantum mechanical phonons [**9**], a more common choice, which we will follow here, is to describe them in the Born-Oppenheimer approximation by adding to the Hamiltonian (1.1) a classical potential of the form

$$\sum_{j=1}^{L} V(w_j)$$

and to minimize, with respect to the w_j, the energy functional

$$\lambda_0(H(\{t(w_j)\})) + \sum_{j=1}^{L} V(w_j) \quad ,$$

where $\lambda_0(H)$ denotes the lowest eigenvalue of H. Often V is taken to be quadratic, but in this paper we will *not* assume that V is quadratic or that the dependence of the t_j on the w_j is linear.

The Peierls Instability [**13**] (discovered also by Fröhlich [**14**] and seemingly independently by Longuet-Higgins and Salem [**15**]) states that for L sufficiently large and U not too large, the minimum will not be attained in a translation invariant configuration of w_j's. By a straightforward computation (exact in the case $U = 0$ or perturbative for small non-zero U) one can show that, for any fixed choice of the function V, there is an L_0 such that for all $L \geq L_0$ the ground state energy of H with

$$w_j = w_0 + (-1)^j \delta \quad , \tag{1.2}$$

for small δ, is lower than with the best choice of $w_j =$ constant. In the context of $(CH)_x$ molecules this was discovered independently by Labhart [**16**] and Ooshika [**17**].

The phenomenon described by (1.2) is called *dimerization* in the physics literature. Unfortunately, this word has quite different connotations in the chemistry literature, but there does not seem to be a universally accepted terminology for (1.2) among chemists. The phrase *bond-alternation* [**15**] would be a more accurate description as far as chemists are concerned. We are obliged to make a choice here, and we shall use "dimerization" — in the hope that chemists will substitute "bond-alternation" for it in their minds. In fact we shall go further and *declare a configuration to be dimerized, even if* (1.2) *holds with* $\delta = 0$, i.e., the w_j's are translation invariant. In other words, a dimerized configuration is one with period-two translation invariance, and this includes period one as a special case. This convention, while a bit unusual, conveniently eliminates awkward locutions.

For the Hückel model ($U = 0$) and for $L = 2 \bmod 4$ (i.e., $L = 6, 10, 14, \ldots$) the dimerization instability was shown very explicitly by Longuet-Higgins and Salem who also estimated the degree of dimerization δ for realistic values of the parameters [**15**]. The physical mechanism for the occurence of lattice distortions is rather simple and quite universal for electron-lattice systems in one dimension. A lattice distortion of period $1/2k_F$ opens up a gap at the Fermi level, thus lowering the energy of the occupied levels. This was a basic ingredient in Fröhlich's theory of superconductivity. The calculations mentioned above show that for small distortions this lowering of the energy exceeds the positive contribution to the total energy of the lattice distortion itself. In the infinite volume limit the elastic energy per bond is quadratic in the parameter δ of (1.2), while the electronic energy per bond decreases by an amount proportional to $\delta^2 \log \delta$ for small δ. As far as we know the first author who mentions this logarithmic behavior is Fröhlich in [**14**].

A common feature of the works mentioned above is that they always show that certain instabilities exist. The question of the "stability of the instabilities" is usually not raised, much less resolved. The main purpose of this work is to study the stability and instability of lattice distortions and to obtain rigorous statements about the true energy minimizing state. Longuet-Higgins and Salem [**15**] raised the question of the possible occurrence of higher periodicities but expected them to be unimportant. We prove that in the case $L = 2 \bmod 4$ (an assumption they made for technical reasons) they were right: *indeed nothing else than periodicity two occurs for* $L = 2 \bmod 4$, *but when* $L = 0 \bmod 4$ *other instabilities may, in fact, occur.*

For the Hückel model with $t = t_0 - \alpha w$ and $V(w) = k(w - a)^2$, Kennedy and Lieb [**18**] showed that the true minimizing configuration is *always* of periodicity two, i.e., w_j is of the form (1.2). Moreover, the minimizing configuration is unique (up to translations). It is remarkable that this result holds for *all even* L, in contrast with what will be proved here for general functions V.

We note parenthetically that the models we study are also used to describe electrons in mesoscopic metallic rings [**19**]. These rings are typically two orders of magnitude larger than the largest annulenes produced in the laboratory so far, and therefore the magnetic fields needed to obtain a flux through the ring of the order of a flux quantum are much smaller and experimentally accessible. The main issue is to calculate the persistent currents in such a ring threaded by a magnetic flux. Depending on the electron number, among other things, these currents can be paramagnetic or diamagnetic. Although most authors assume uniform hoppings t for this problem, there is an intimate connection between these persistent currents and the stability of dimerized configurations of t's.

In order to proceed to a precise formulation of our results it is first necessary to confront some possibly confusing questions about the phases of the t_j's. Let us write

$$t_j = |t_j| \exp[i\theta_j]$$

with $-\pi < \theta_j \leq \pi$. We note, first, that by a simple unitary gauge transformation of the type $c_{j\sigma} \to \exp[i\varphi_j] c_{j\sigma}$ and $c^\dagger_{j\sigma} \to \exp[-i\varphi_j] c^\dagger_{j\sigma}$, the operators $n_{j\sigma}$ and the energy levels of H are unchanged, but the t_j's change to $t_j \to t_j \exp[i(\varphi_j - \varphi_{j+1})]$. Consequently, the energy levels depend *only* on the "total flux", Φ, of the t_j's defined by

$$\Phi = \text{argument}(\prod_{j=1}^{L} t_j) \quad ,$$

with $-\pi < \Phi \leq \pi$.

The next consideration comes from the physics of our model. The t_j's are real, unless there is a superimposed magnetic field, in the absence of which each $\theta_j = 0$ or π, depending on whether t_j is positive or negative. Both signs can occur. Furthermore, it is understood that the t_j's remain close to some nonzero value in the physically realistic situation. Without loss of generality we can choose this value to be positive. With this in mind, we shall assume that the elastic energy, as a function of t, defined by

$$f(|t|) \equiv \inf\{V(w) \mid t(w) = t\} \quad ,$$

depends only on $|t|$ and not on the sign of t. (We will impose below in (1.6) some other very mild physical conditions on f.) This is not to say that negative t's will not be permitted. They will — as we explain next.

Our procedure will be to study the total energy

$$\mathcal{E}_L(\{t_j\}) \equiv \lambda_0(H(\{t_j\})) + \sum_{j=1}^{L} f(|t_j|) \quad , \tag{1.3}$$

and to evaluate its minimum

$$E_L \equiv \min_{\{t_j\}} \mathcal{E}_L(\{t_j\}) \quad , \tag{1.4}$$

where the minimum is taken over all choices of $\{|t_j|\}$ *as well as* the phases $\{\theta_j\}$. Thus, we allow negative t_j's and give them the same elastic energy as $|t_j|$. Since the t_j's are not expected to pass through zero in the physical case, this is no real restriction. In terms of the t_j, dimerization means that the configurations minimzing $\mathcal{E}_L(\{t_j\})$ are of the form

$$t_j = t_0 + (-1)^j \delta \quad . \tag{1.5}$$

It will turn out that for all L our theorems show that the energy minimzing t_j's are real (modulo a gauge transformation). But for $L = 0 \bmod 4$ an odd number of them *must* be negative for an energy minimizer — thereby precluding a dimerized state. If, on the other hand, we wish to attribute the occurrence of an odd number of negative t_j's to the presence of an external magnetic field then we can say that a dimerized state minimizes the energy in the presence of a field of flux π. Given that no such field is really present, we will have to conclude that the energy mimimum will not be a dimerized state when $L = 0 \bmod 4$. In this case we can redefine our problem by restricting the minimum in (1.4) to positive t_j's. Do we get a dimerized state then? We do not know the general answer but we have some conjectures about this question. If $f(t) = k(t-a)^2$, as in **[18]**, we know that a dimerized state is, indeed, the minimum.

The physical conditions we impose on f are

$$\begin{aligned} &\text{i) } f \text{ is continuous.} \\ &\text{ii) } f(t) \geq Ct, \text{ for large } t \text{ and for some constant } C > 4. \end{aligned} \tag{1.6}$$

The continuity of f is not really necessary for the validity of our results. In fact in the Appendix (Lemma 13) we show that f can always be replaced with a convex (and hence continuous) function without changing the minimizing configurations. Property ii) is necessary to have a stable minimum at all, e.g., to prevent the molecule from collapsing to a point.

We minimize the ground state energy $\mathcal{E}_L$ not only with respect to the parameters t_j but *also* with respect to the number of electrons. In Section 2 we prove that if $U \neq 0$ and all t_j are real, the ground states of (1.1) will in fact necessarily have $N = L$. In this case all results below are equally valid for minimization of the energy with the particle number fixed at half-filling. The condition $U \neq 0$ is necessary in the case of rings of size $L = 0 \bmod 4$, for with $U = 0$ the model with translation invariant t's has ground states with particle number ranging from $L = -2$ to $L + 2$, due to zero eigenvalues of the one-particle Hamiltonian.

Relation with the Flux-Phase Problem.
The minimization with respect to the flux Φ of $\mathcal{E}_L(\{t_j\})$, for fixed $|t_j|$, is a generalization of the so-called flux-phase problem [**20,21**] for rings. In the case $U = 0$ (as in the original formulation of this problem), but arbitrary, fixed, positive $\{t_j\}$, this problem was solved by Lieb and Loss [**22**]. The arguments of this paper provide a way of solving the problem for rings and all values of U (Corollary 8). For rings of length $L = 2 \bmod 4$ the optimal ($\equiv$ energy minimizing) flux is 0. When $L = 0 \bmod 4$, the optimal flux is $\varphi = \pi$. This can be extended to higher dimensions [**23**] when some geometric periodicity is present. In particular, [**23**] proves the conjecture that the optimal flux for the Hubbard model on the two-dimenisonal square lattice is π through each plaquette.

Main Results.
The following theorem, which we prove in Section 3, says that, when $L = 2 \bmod 4$ and the flux is zero and when $L = 0 \bmod 4$ and the flux is π, the Peierls instability is itself stable in the sense that no other lattice distortions than period two can occur. The theorem does *not* state that distortion always happens. Depending on the parameters in the Hamiltonian, the function f in particular, the energy minimzing configuration may or may not be translation invariant. In real molecules both situations occur. Benzene, e.g., has all $C - C$ bond lengths equal (within the precision of today's measurements and in agreement with the analysis of Labhart [**16**] and Ooshika [**24**]), while for large rings or long chains the Peierls instability will necessarily lead to two different bond lengths.

1 Theorem (Minimizing configurations).

i) If $L = 2 \bmod 4$, the minimum of $\mathcal{E}_L$ is attained in a dimerized configuration of the form (1.5) *in which the t_j's are all positive (or all negative).*

ii) If $L = 0 \bmod 4$, the minimum of $\mathcal{E}_L$ is attained configuration in which the $|t_j|$'s satisfy (1.5) *but the flux Φ equals π.*

That the cases $L = 2 \bmod 4$ and $L = 0 \bmod 4$ behave differently with respect to the flux was noted a long time ago (see e.g. the "Hückel rule" in [**2**].) The $U = 0$ one-electron problem has zero-energy states when $L = 0 \bmod 4$ but not when $L = 2 \bmod 4$. In the first case this leads to diamagnetic, in the second case to paramagnetic response to magnetic fields, as was noted in [**3**] and as is observed experimentally in the annulenes [**25**].

2 Theorem (Uniqueness). *If there is only one (up to translation and gauge transformations) dimerized configuration satisfying the conclusion of Theorem 1, then there are no other energy minimizing configurations.*

We define three additional minimization problems for the $L = 0 \bmod 4$ case.

- *Zero-flux problem:* We restrict the minimization in (1.4) to those $\{t_j\}$ with zero flux, i.e., $\Phi = 0$.
- *Period-two problem:* In addition to $\Phi = 0$ we make the further restriction that the t_j's must be dimerized.
- *The infinite-chain problem:* Let $d(x, y)$ denote the dimerized configuration with $t_{2j+1} = x$ and $t_{2j} = y$, and minimize the energy per site defined by

$$e(x, y) = \lim_{L\to\infty} \frac{1}{L}\mathcal{E}_L(d(x, y)) \quad . \tag{1.7}$$

The minimum energy in the first case is denoted by E_L^0, and the t_j's by t_j^0. The second energy is denoted by $E^0_{L,\mathrm{dimer}}$ and the t_j's by $t^0_{j,\mathrm{dimer}}$. Clearly

$$E^0_{L,\mathrm{dimer}} \geq E_L^0$$

and one of our conjectures below concerns the case of equality. The following, however, shows that the three problems become asymptotically the same (to within two powers of L^{-1}, instead of merely one) as $L \to \infty$.

3 Theorem (Asymptotic dimerization).

i) Assume that there is a unique energy minimizing dimerized configuration $d(x, y)$, $x \geq y$, for the infinite-chain problem. Then any sequence of minimizing configurations $\{t_j^0\}$ of the zero-flux problem converges to a dimerized configuration as $L \to \infty$. Namely,

$$\lim_{L\to\infty} \max_j |t_j^0 - t^0_{j,\mathrm{dimer}}| = \lim_{L\to\infty} \max_j |t_j^0 - d(x, y)_j| = 0 \quad ,$$

where we have adopted the convention that t_1 is the largest of the t_j's for all configurations.

ii) For any even L, the energies satisfy

$$0 \leq E_{L,\mathrm{dimer}} - E_L^0 \leq \mathit{constant} \times L^{-1} \quad .$$

In section 5 we discuss the situation of finite rings of length $L = 0 \bmod 4$. Instabilities other than period-two can exist for arbitrarily large rings if the function f is chosen appropriately. An optimally dimerized ring of size $L = 0 \bmod 4$ can have other instabilities and it seems that the strongest of those actually has wavelength $= L$, and is not, as one could have expected, of period 4 or some other higher periodicity. We illustrate this with an explicit example of a ring of 8 sites for which the minimum is not period 2. A perturbative analysis indicates that the conditions on f for a further instability to occur become more stringent as the system becomes larger. In particular the dimerization itself has to be smaller as L becomes bigger. This leads us to the following two conjectures:

Conjecture 1. For every $L = 0 \bmod 4$ there exists a function f (depending on L), satisfying conditions i) and ii) in (1.6), such that the energy minimizing configurations for the zero-flux problem are *not* period two.

Conjecture 2. For any fixed f satisfying (1.6), and such that there is a unique minimum for the infinite-chain problem, there is a critical size L_c such that for all even $L \geq L_c$ all zero-flux minima are period two.

The Spin-Peierls Problem.

Another closely related question is the spin-Peierls problem. For U large, and half-filling, the Hubbard model reduces to the Heisenberg antiferromagnetic spin chain in second order perturbation theory [**26**]. The spin chain also has an instability when coupled to lattice distortions, as was pointed out by Chesnut [**27**] and by Beni and Pincus [**28,29**]. More explicitly one looks for the configurations of coupling constants J_{ij} that minimize the smallest eigenvalue of the Hamiltonian:

$$H_\Lambda = \sum_{<i,j>} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{<i,j>} f(J_{ij}) \quad , \tag{1.8}$$

where the sum is over nearest neighbour pairs in a finite subset Λ of the hypercubic lattice, and $f(J_{ij})$ is the elastic energy as before. In one dimension Cross and Fisher [**30**] computed the exponent governing the ground state energy density $e(\delta)$ of the system with alternating couplings:

$$J_j = 1 + (-1)^j \delta \quad ,$$

with $J_j \equiv J_{j,j+1}$. They found that, up to logarithmic corrections,

$$|e(\delta) - e(0)| \sim -|\delta|^{4/3} \quad .$$

Numerical confirmation of this exponent and evidence for a logarithmic correction was reported in [**31**]. The important point here is that $4/3 < 2$, which implies the instability of the translation invariant configurations under period 2 perturbations, provided f has a finite second derivative. It was recently proved that this exponent is identical to a critical exponent of the two dimensional 4-state Potts model [**32**].

The question addressed in this paper is again to determine the nature of the minimizing configurations. It turns out that the true minimum is dimerized for any (even) system size and in any dimension. *The* 2 mod 4 *versus* 0 mod 4 *dichotomy does not arise for the Heisenberg model!*

4 Theorem (Dimerization for spin-Peierls). *Let $\Lambda \subset \mathbb{Z}^d$ be a rectangular box of even size in all coordinate directions and with periodic boundary conditions. Then there is an energy minimizing configuration of J_{ij}'s which is of periodicity 2 in all coordinate directions.*

This theorem prompts one more conjecture.

Conjecture 3. Suppose that a minimizer for the zero-flux problem for some f and $L = 0 \bmod 4$ and some $U_0 \geq 0$ is a dimerized state. Then for every $U > U_0$ there is a dimerized minimizer for the zero-flux problem with the same f and L. In particular, the truth of this conjecture, when combined with the $U = 0$ result in **[18]**, would imply that, with a quadratic f, dimerization always occurs, even in the $L = 0 \bmod 4$ case.

Extensions of the results presented in this paper.

1) It has been argued that the Hubbard on-site repulsion does not describe the Coulomb interaction between the electrons accurately enough (for a discussion see e.g. the reviews on this topic in **[33]** and references therein). While the Hubbard term alone, when not too large, seems to have the effect of enhancing the dimerization **[34]**, taking into account some nearest neighbour interaction terms Kivelson, Su, Schriefer, and Heeger **[35]** found that the Coulomb repulsion in fact suppresses the dimerization in polyacetylene. Without entering into this discussion here we would like to point out that without substantial modification one can prove the results of Theorem 1 and Theorem 2 for a Hamiltonian that includes a repulsive nearest-neighbour interaction of the form

$$\sum_j W(t_j)(n_j - 1)(n_{j+1} - 1)$$

The -1's are inserted to keep the chemical potential tuned at half-filling. We require $W(t) \geq 0$, but no assumption on the dependence of W on t is needed. Theorem 1 holds unchanged, but we can extend the proof that the grand canonical ground states are necessarily half-filled only under the additional condition that $W(t_{j-1}) + W(t_j) < U_j$, for all t's in the relevant range. Nearest neighbour exchange terms and certain longer range interactions can also be treated.

2) Instead of a homogeneous on-site repulsion it is sometimes more realistic to have different U for different (classes of) sites, e.g. in a periodic manner. Theorem 1 extends to such situations in the following sense: the minimum energy will be attained in a configuration of t_j which is invariant under all reflections through planes that intersect two oppossite bonds on the ring (as indicated by a dashed line in Figure 1) and that leave the configuration of the U_i invariant. As an example consider [18]-annulene. Of the 18 hydrogens in this molecule 6 reside inside the ring and 12 outside, according to the pattern: 1 inside, 2 outside, 1 inside, etc. A possible way of taking the effect of this periodic configuration of H-atoms into account, is to add a periodic one-particle potential to the Hamiltonian. In the present example this potential would take two different values and depend on the site according to the pattern: $(v_i) = (v_1, v_1, v_2, v_1, v_1, \ldots)$. Our general result then implies an energy minimizing configuration of $C - C$ bonds of the form $ABCACBABCACB\ \cdots$. The observed bond lengths in [18]-annulene indeed satisfy this pattern (they are $A = 1.419$Å, $B = 1.382$Å,$C = B$ **[25]**.)

3) Hubbard models with spin-dependent hoppings, i.e., $t_j = |t_j| m_j, m_j \in \mathrm{SU}(2)$, have been considered in the literature in order to study the effects of spin-orbit coupling **[36,37,38]**. By virtue of the SU(2) gauge symmetry of the Hamiltonian one can diagonalize the spin dependence of the hoppings up to an SU(2) flux, which is defined up to an SU(2) transformation

by the matrix $M = m_1 m_2 m_3 \cdots m_L$. The methods of this paper can be used to prove the existence of a minimizer having dimerization and $M = \mathbb{1}$ when $L = 2 \bmod 4$ and when $L = 0 \bmod 4$ a minimizer has $M = -\mathbb{1}$ and dimerization. This is completely analogous to the U(1) case treated in Theorem 1.

4) Mattis and Langer [**39**] introduced a simple model to study the interaction between the electrons and a phonon instability of the Peierls type as a function of the temperature. Our methods can also be used to prove that in this model the electron state has periodicity two and that its correlations indicate dimerization. For a rigorous study of the Kohn anomaly, which accompanies the phase transition in the Mattis-Langer model, see [**40**].

Generalizations that are not considered in this work include the interaction between the electrons and lattice in excited states, the effects of doping, and higher dimensional models. Low-lying electronic excited states can induce further (e.g. soliton-like) distortions of the lattice [**9,41,42**]. In doped polyacetylene an interesting semiconductor-metal transition occurs [**43**]. Away from half-filling, instabilities other than period-two will naturally develop (see e.g. [**44**] and references therein). In two dimensions, e.g., on a square lattice, $2k_F$ instabilities may develop either in the coordinate directions or in the diagonal directions [**45,46**]. This may be related to the non-period-two instabilities that can occur in rings whose size is a multiple of 4, e.g., in the elementary plaquettes of the square lattice. Another new feature of higher dimensions is that the breaking of translation invariance can occur at non-zero temperature. This has been rigorously shown to occur in the Falicov-Kimball model [**47,48**] and in the Holstein model [**49**].

2. THE GRAND CANONICAL HUBBARD MODEL AT HALF-FILLING

In the definition of the energy functional (1.3) we used the lowest eigenvalue of the grand canonical Hubbard Hamiltonian at half-filling. Our goal in this section is to prove that the corresponding ground state necessarily has $N = L$ if we assume the t_j's are real (as will later be shown to be the case). It is then obvious that minimization of the energy with respect to the parameters t_j *and* the number of electrons, produces exactly the same minimizing configurations as the restricted mimimization with the particle number fixed at $N = L$. The arguments in this section are not restricted to one dimension. We believe they are interesting in their own right and can be of interest in a more general context. Therefore, we temporarily consider a more general setup on a general finite lattice Λ, the number of whose lattice sites is denoted by $|\Lambda|$.

Consider the grand canonical Hubbard Hamiltonian (1.1) for spin 1/2 fermions on Λ, and with arbitrary chemical potential μ:

$$H = -\sum_{i,j\in\Lambda}\sum_{\sigma=\uparrow,\downarrow} t_{ij} c_{j\sigma}^\dagger c_{i\sigma} + \sum_{j\in\Lambda} U_j (n_{j\uparrow} - \mu)(n_{j\downarrow} - \mu)$$

The t_{ij} are asssumed (in this section only) to be real and symmetric, i.e $t_{ij} = t_{ji}$. Λ is assumed to be connected, i.e., given i and j in Λ we can find a sequence $i = i_1, i_2, \ldots, i_m = j$ such that $t_{i_1,i_2} t_{i_2,i_3} \cdots t_{i_{m-1},i_m} \neq 0$. The U_j and μ are also real parameters. As before the dependence of H on its parameters will be made explicit with a notation of the type H_μ,

$H(\{t_{ij}\})$, $H_\mu(\{t_{ij}\},\{U_j\})$ etc. When H appears without subscript the chemical potential is $\mu = 1/2$, corresponding to half-filling.

The spin-up and spin-down particle number operators are defined by

$$N_\sigma = \sum_{j\in\Lambda} n_{j\sigma}$$

where $\sigma = \uparrow, \downarrow$ and $n_{j\sigma} = c^\dagger_{j\sigma} c_{j\sigma}$. Note that $N_\uparrow$ and $N_\downarrow$ each commute with H, and hence their eigenvalues are good quantum numbers. H also commutes with the total-spin operators (which generate the global spin rotations) given by

$$S^+ = \sum_j c^\dagger_{j\uparrow} c_{j\downarrow}, \quad S^- = \sum_j c^\dagger_{j\downarrow} c_{j\uparrow}, \quad S^3 = \frac{1}{2}(N_\uparrow - N_\downarrow)$$

Therefore, by applying S^+ or S^- an appropriate number of times, one can transform any ground state of H into a ground state with

$$N_\uparrow - N_\downarrow = \begin{cases} 0 & \text{if } N \text{ is even} \\ \pm 1 & \text{if } N \text{ is odd} \end{cases} \tag{2.1}$$

We say that Λ and t are bipartite if the sites of Λ can be written as the disjoint union of two subsets; i.e., $\Lambda = \Lambda_A \cup \Lambda_B$, in such a way that the matrix t of hopping matrix elements respects this structure, namely $t_{ij} = 0$ if $i \in \Lambda_A$ and $j \in \Lambda_A$ or if $i \in \Lambda_B$ and $j \in \Lambda_B$. In this case the Hamiltonians $H_{1/2}(\{t_{ij}\},\{U_j\})$ and $H_{1/2}(\{t_{ij}\},\{-U_j\})$ are unitarily equivalent, i.e at half-filling ($\mu = 1/2$) a global sign change of the potential does not affect the spectrum. A unitary transformation implementing this equivalence is the particle-hole transformation mapping

$$\begin{gathered} c^\dagger_{j\uparrow} \longrightarrow \varepsilon(j) c_{j\uparrow}, \quad c_{j\uparrow} \longrightarrow \varepsilon(j) c^\dagger_{j\uparrow} \\ c^\dagger_{j\downarrow} \longrightarrow c^\dagger_{j\downarrow}, \quad c_{j\downarrow} \longrightarrow c_{j\downarrow} \end{gathered}$$

where $\varepsilon(j) = 1$ for $j \in \Lambda_A$ and $\varepsilon(j) = -1$ for $j \in \Lambda_B$. By the same transformation the spin operators are mapped into the so-called *pseudospin* operators defined by

$$\tilde{S}^+ = \sum_j \varepsilon(j) c_{j\uparrow} c_{j\downarrow}, \quad \tilde{S}^- = \sum_j \varepsilon(j) c^\dagger_{j\downarrow} c^\dagger_{j\uparrow}, \quad \tilde{S}^3 = \frac{1}{2}(|\Lambda| - N_\uparrow - N_\downarrow)$$

These operators therefore also commute with the Hamiltonian, and they also commute with the spin operators and generate an additional SU(2) symmetry. Under the particle-hole transformation $N_\uparrow$ and $N_\downarrow$ are transformed into $|\Lambda| - N_\uparrow$ and $N_\downarrow$ respectively. It is then obvious that by applying $\tilde{S}^\pm$ to any ground state we can obtain a ground state with

$$N_\uparrow + N_\downarrow = \begin{cases} |\Lambda| & \text{if } N - |\Lambda| \text{ is even} \\ |\Lambda| \pm 1 & \text{if } N - |\Lambda| \text{ is odd} \end{cases} \tag{2.2}$$

As the spin and pseudospin operators commute (2.1) and (2.2) can be realized simultaneously. For an even bipartite lattice and $\mu = 1/2$ this implies that there is a ground state of H with $N_\uparrow = N_\downarrow = |\Lambda|/2$ or $N_\uparrow = N_\downarrow \pm 1 = |\Lambda|/2$.

¿From the next lemma it will follow that if in addition all U_j are nonvanishing and of the same sign, *all* ground states have even particle number and satisfy $N_\uparrow = N_\downarrow = |\Lambda|/2$. Note that the Lemma itself does not require Λ to be bipartite.

5 Lemma. *If all t_{ij} are real and $U_j \leq 0$ for all j, then the ground state space of $H(\{t_{ij}\}, \{U_j\})$ contains a state with $N_\uparrow = N_\downarrow$. If $U_j < 0$ for all j, all groundstates satisfy $N_\uparrow = N_\downarrow$. In particular the total number of particles in the ground state is even and the total spin is zero.*

Proof : We can introduce new operators $\hat{c}_{i,\sigma}$ defined by

$$\hat{c}_{j,\uparrow} = c_{j,\uparrow}, \quad \hat{c}_{j,\downarrow} = (-1)^{N_\uparrow} c_{j,\downarrow}$$

H has then the same form in terms of the $\tilde{c}$'s as in terms of the c's, but now the $\hat{c}^{\#}_{j,\downarrow}$ commute with the $\hat{c}^{\#}_{j,\uparrow}$.

Our Hamiltonian is now an operator on $\mathcal{H}_\uparrow \otimes \mathcal{H}_\downarrow$, and can be written in the form

$$H = T \otimes \mathbb{1} + \mathbb{1} \otimes T + \sum_{i \in \Lambda} U_j (n_j - \mu) \otimes (n_j - \mu)$$

where $T = -\sum_{i,j \in \Lambda} t_{ij} c_j^\dagger c_i$. (Because spin $\uparrow$ and spin $\downarrow$ operators act identically on different tensor factors in the Hilbert space, we can omit the spin index.) T and the n_j are real in the canonical basis of localized particles. Therefore we can apply Lemma 14 of the appendix and the discussion thereafter to conclude that H has a ground state with $N_\uparrow = N_\downarrow$.

If $U_j < 0$ for all i, there cannot be a ground state with $N_\uparrow \neq N_\downarrow$. Indeed the last statement of Lemma 14 implies that for any ground state Ω

$$U_j \langle \Omega \mid (n_{j,\uparrow} - \mu) \Omega \rangle = U_j \langle \Omega \mid (n_{j,\downarrow} - \mu) \Omega \rangle$$

If $U_j < 0$ this implies $N_\uparrow = N_\downarrow$. **Q.E.D.**

6 Lemma. *If all t_{ij} are real and bipartite, $|\Lambda_A| = |\Lambda_B|$, and either all $U_j > 0$ or all $U_j < 0$. Then the ground state of H with $\mu = 1/2$ is unique and has $N_\uparrow = N_\downarrow = |\Lambda|/2$.*

Proof : It is sufficient to consider the case of all $U_j > 0$. The case $U_j < 0$ then follows because the particle-hole transformation changes the sign of the U_j, and the properties $N_\uparrow = |\Lambda|/2$ and $N_\downarrow = |\Lambda|/2$ are unchanged under the transformation. Let us therefore consider the case $U_j > 0$, for all j.

We first apply Lemma 5 to the particle-hole transformed Hamiltonian which has all $U_j < 0$. This tells us that $N_\downarrow = |\Lambda| - N_\uparrow$ in all ground states. In particular the total number of particles is $|\Lambda|$ which, by assumption, is even. Then, by Theorem 2 of **[50]** (the grand-canonical version at half-filling does not need the homogeneity of the potential) and the assumptions on the lattice, $N_\uparrow = N_\downarrow = |\Lambda|/2$. [Note: Theorem 2 of **[50]** requires $U_j =$ constant. That is the case when the interaction is $n_{j\uparrow}n_{j\downarrow}$ as in [**50**]. If we use the formulation of (1.1), however, with $(n_{j\uparrow}-1/2)(n_{j\downarrow}-1/2)$, the same proof works without the need of constant U_j.] **Q.E.D.**

For translation invariant t_{ij} on regular lattices the case $U_j \equiv 0$ is of course exactly solvable. It is rather straightforward in such cases to determine the ground state degeneracy "by hand". The ground state is unique if and only if the eigenvalues of the matrix (t_{ij}) are all non-zero.

It is straightforward to extend Lemma 5 to Hamiltonians that include interactions of the form

$$F(\{n_{j,\uparrow}\})+F(\{n_{j,\downarrow}\})-\sum_{\alpha} G_\alpha(\{n_{j,\uparrow}\})G_\alpha(\{n_{j,\downarrow}\})$$

for arbitrary real functions F and G of the local particle numbers. One can use this to prove a slightly weaker form of Lemma 6 for a class of models with an additional term of the form

$$-\sum_{ij} W_{ij}(n_i-1)(n_j-1)$$

added to the Hamiltonian H. For these models our methods also prove that

i) if $W_{ij}\geq 0$ and $(U_j-\sum_i W_{ij})\geq 0$, for all j, then there is a ground state with $N_\uparrow = N_\downarrow = |\Lambda|/2$.

ii) if $W_{ij}\geq 0$ and $(U_j-\sum_i W_{ij}) > 0$, all ground states have $N_\uparrow = N_\downarrow = |\Lambda|/2$.

3. GENERAL RESULTS BASED ON REFLECTION POSITIVITY; PROOFS OF THEOREMS 1 AND 4

We now return to the half-filled Hubbard model ($N=|\Lambda|$) on a ring of even length $|\Lambda| = L$. It will be convenient to express the dependence of the energy functional on $\{t_j\}$ in a more explicit way. We write

$$\mathcal{E}_L(t^{(l)},t^{(m)},t^{(r)}) = \lambda_0(H(\{t_j\})) + \sum_{j=1}^{L} f(|t_j|) \quad ,$$

where $t^{(l)}, t^{(r)}$, and $t^{(m)}$ denote a partition of the *complex* t_j's (with t_j^* denoting the complex conjugate of t_j) into three groups as follows (also see Figure 1):

$$t^{(r)} = (t_1,\ldots,t_{L/2-1}), \quad t^{(m)} = (t_L, t_{L/2}), \quad t^{(l)} = (t_{L-1},\ldots,t_{L/2+1}) \quad .$$

The reflection of a configuration $(t^{(l)},t^{(m)},t^{(r)})$ through the plane intersecting the bonds $\{L,1\}$ and $\{L/2, L/2+1\}$ is the configuration $(t^{(r)},t^{(m)},t^{(l)})$, i.e., with $t^{(l)} \leftrightarrow t^{(r)}$.

Throughout this section we assume a constant potential $U_j = U$. The following lemma can be formulated to include non-constant potentials but this is not needed for our purposes.

7 Lemma. *Assume a constant potential $U_j = U$. If $L = 2 \bmod 4$, assume that $t_{L/2}$ and t_L are real and nonnegative. If $L = 0 \bmod 4$, assume that $t_{L/2} \geq 0$ and $t_L \leq 0$. The other t_j are allowed to be arbitrary complex numbers. Then the energy functional satisfies*

$$\mathcal{E}_L(t^{(l)}, t^{(m)}, t^{(r)}) \geq \frac{1}{2}\left(\mathcal{E}_L(t^{(l)}, t^{(m)}, t^{(l)*}) + \mathcal{E}_L(t^{(r)*}, t^{(m)}, t^{(r)})\right) \quad . \tag{3.1}$$

Proof : As in the proof of Lemma 5 we consider the Hamiltonian (1.1) as acting on $\mathcal{H}_\uparrow \otimes \mathcal{H}_\downarrow$, which amounts to considering operators referring to opposite spins as commuting. For $\sigma = \uparrow, \downarrow$ define a set of "spin" operators using a Jordan-Wigner transformation as follows:

$$\begin{aligned} S^3_{j,\sigma} &= c^\dagger_{j,\sigma} c_{j,\sigma} - \tfrac{1}{2} \quad , \quad \mathbf{S}_{j,\sigma} = 2S^3_{j,\sigma} \quad , \\ S^+_{j,\sigma} &= \mathbf{S}_{1,\sigma} \cdots \mathbf{S}_{j-1,\sigma} c^\dagger_{j,\sigma} \quad , S^-_{j,\sigma} = \mathbf{S}_{1,\sigma} \cdots \mathbf{S}_{j-1,\sigma} c_{j,\sigma} \quad . \end{aligned}$$

With these definition and the anticommutation relations of the $c_{i,\sigma}$ and $c^\dagger_{i,\sigma}$ it is straigthforward to check that $S^3_{i,\sigma}, S^+_{i,\sigma}$, and $S^-_{i,\sigma}$ satisfy the standard SU(2) commutation relations and that they commute for different indices i, σ. In terms of these operators, and using the commutation relations, the Hamitonian can be written as

$$\begin{aligned} H = &\sum_{j=1}^{L-1} \sum_{\sigma=\uparrow,\downarrow} t_j S^+_{j+1,\sigma} S^-_{j,\sigma} + \text{ h.c. } + U \sum_{j=1}^{L} S^3_{j,\uparrow} S^3_{j,\downarrow} \\ &t_L \sum_{\sigma=\uparrow,\downarrow} S^+_{1,\sigma}(\mathbf{S}_{1,\sigma} \cdots \mathbf{S}_{L,\sigma}) S^-_{L,\sigma} + \text{ h.c.} \quad . \end{aligned}$$

By performing a rotation by π about the 2-axis at every other site and for both $\sigma = \uparrow$ and $\sigma = \downarrow$ we find that this spin Hamiltonian is unitarily equivalent to:

$$\begin{aligned} \tilde{H} = &\sum_{j=1}^{L-1} \sum_{\sigma=\uparrow,\downarrow} -t_j S^+_{j+1,\sigma} S^+_{j,\sigma} + \text{ h.c. } + \sum_{j=1}^{L} U_j S^3_{j,\uparrow} S^3_{j,\downarrow} \\ &+ (-1)^{L/2} t_L \sum_{\sigma=\uparrow,\downarrow} S^+_{1,\sigma}(\mathbf{S}_{1,\sigma} \cdots \mathbf{S}_{L/2,\sigma}) S^+_{L,\sigma}(\mathbf{S}_{L,\sigma} \cdots \mathbf{S}_{L/2+1,\sigma}) + \text{ h.c.} \quad . \end{aligned}$$

Under the conditions stated in the proposition $t_{L/2} \geq 0$ and $(-1)^{L/2} t_L \leq 0$. We can now apply Lemma 14 of the appendix to $\tilde{H}$ with

$$\begin{aligned} A &= -\sum_{j=1}^{L/2-1} \sum_{\sigma=\uparrow,\downarrow} t_j S^+_{j+1,\sigma} S^+_{j,\sigma} + \text{ h.c. } + U \sum_{j=1}^{L/2} S^3_{j,\uparrow} S^3_{j,\downarrow} \quad , \\ B &= -\sum_{j=L/2+1}^{L-1} \sum_{\sigma=\uparrow,\downarrow} t_j S^+_{j+1,\sigma} S^+_{j,\sigma} + \text{ h.c. } + U \sum_{j=L/2+1}^{L} S^3_{j\uparrow} S^3_{j\downarrow} \quad , \\ C_1 \otimes C_1 &= t_{L/2} S^+_{L/2+1,\uparrow} S^+_{L/2,\uparrow} \quad , \\ C_2 \otimes C_2 &= |t_L| S^+_{1,\uparrow}(\mathbf{S}_{1,\uparrow} \cdots \mathbf{S}_{L/2,\uparrow}) S^+_{L,\uparrow}(\mathbf{S}_{L,\uparrow} \cdots \mathbf{S}_{L/2+1,\uparrow}) \quad , \end{aligned}$$

and six more terms $C_i \otimes C_i$, $i = 3, \ldots, 8$, which are equal to $C_1 \otimes C_1$ and $C_2 \otimes C_2$ with $\uparrow$ replaced by $\downarrow$ and the hermitian conjugates of these operators. This gives us the inequality of the lemma for the lowest eigenvalue of H. The elastic energy terms in the functional $\mathcal{E}_L$

add up to the same contribution on both sides of the inequality and therefore can be included trivially. **Q.E.D.**

Proof of Theorem 1 :
First we prove that the minimum of $\mathcal{E}_L$ is attained in a configuration of t_j with total flux Φ when $L = 2 \bmod 4$, and with $\Phi = \pi$ when $L = 0 \bmod 4$. Let $\{t_j\}$ be minimizing. Due to the invariance of the ground state energy of H under gauge transformations, the energy functional $\mathcal{E}_L$ defined in (1.3) depends only on $\{|t_j|\}$ and Φ. Hence, for any set of t_j's there are t'_j such that $\mathcal{E}_L(\{t_j\}) = \mathcal{E}_L(\{t'_j\})$ and $t'_{L/2}$ and t'_L are real and have the correct sign for application of Lemma 7. The two configurations in the right side of (3.1) have flux $\Phi = \text{argument}(t'_{L/2}t'_L)$ which, by assumption, takes the values stated in the theorem. Because $\{t_j\}$ is minimizing, (3.1) must be an equality. Therefore the two configurations on the right side must be minimizers of $\mathcal{E}_L$, but then both have the correct flux, 0 or π.

Next we show that in both cases the minimum of $\mathcal{E}_L$ is attained in a configuration with $\{|t_j|\}$ dimerized. For any configuration $(t^{(l)}, t^{(m)}, t^{(r)})$ of real t_j's and $t^{(m)}$ of the right signs, (3.1) implies that either $(t^{(l)}, t^{(m)}, t^{(l)})$ or $(t^{(r)}, t^{(m)}, t^{(r)})$ has at least as low an energy and has at least as many pairs of identical $|t_j|$'s. In particular this shows that $\mathcal{E}_L$ is minimized in a configuration with $|t_j| = |t_{j+2}|$ for $j = L/2 - 1$ and $j = L - 1$. Because $\mathcal{E}_L$ is translation invariant the argument above can be repeated to show that there is a minimizing configuration with $|t_j| = |t_{j+2}|$ for all j, which is the desired result. **Q.E.D.**

Lemma 7 also permits us to solve the flux phase problem for even rings with $U \neq 0$.

8 Corollary. *Let $U_j \equiv U$ and let $\{t_j\}$ be a fixed configuration of nonnegative t_j's. Then the minimum of $\mathcal{E}_L$, varying over the total flux Φ alone, is attained for $\Phi = 0$ if $L = 2 \bmod 4$ and for $\Phi = \pi$ if $L = 0 \bmod 4$.*

Proof of Theorem 4 :
The Heisenberg antiferromagnet on an arbitrary bipartite lattice is reflection positive [**51**]. This implies, via Lemma 14, the following inequality, analogous to Lemma 7:

$$\begin{aligned}
&\lambda_0(H_{\text{Heis.}}(\{J_{ij}^{(l)}, J_{ij}^{(m)}, J_{ij}^{(r)}\}) \\
&\geq \frac{1}{2}\left(\lambda_0(H_{\text{Heis.}}(\{J_{ij}^{(l)}, J_{ij}^{(m)}, J_{ij}^{(l)}\}) + \lambda_0(H_{\text{Heis.}}(\{J_{ij}^{(r)}, J_{ij}^{(m)}, J_{ij}^{(r)}\})\right) \quad ,
\end{aligned}$$

where $\{J_{ij}^{(l)}, J_{ij}^{(m)}, J_{ij}^{(r)}\}$ denotes a partition of the coupling constants into three groups: the $J_{ij}^{(l)}$ are the couplings on the bonds to the left of any reflection plane of the lattice, the $J_{ij}^{(m)}$ are the couplings on the bonds intersected by the reflection plane, and the $J_{ij}^{(r)}$ are the coupling to the right of the plane. Using this inequality Theorem 4 is then proved in the same way as Theorem 1, but this time there is no need to distinguish between $L = 0 \bmod 4$ and $L = 2 \bmod 4$ — or even to restrict ourselves to one dimension. **Q.E.D.**

4. ASYMPTOTIC DIMERIZATION FOR $L = 0 \bmod 4$; PROOFS OF THEOREMS 2 AND 3

Even though finite rings of length $L = 0 \bmod 4$ can do more complicated things than dimerize (see Section 5 for a discussion of counterexamples), they do dimerize asymptotically. To be precise, for a fixed f, satisfying conditions i) and ii) of (1.6), for which the infinite ring has a unique energy minimizing configuration among the configurations of period 2, any sequence of minimizers for finite rings has to approach that dimerized configuration uniformily when $L \to \infty$, i.e., any nearest pair of $|t_j|$'s converges to the pair occurring in the infinite volume dimerized configuration. The aim of this section is to prove this statement, which is Theorem 3 i). At the same time we will also supply the proofs of Theorem 2 and Theorem 3 ii).

In contrast to the previous section, here we will always consider minimization of the energy over arbitrary configurations of $|t_j|$, but with constant flux Φ. For this purpose it is convenient to introduce an explicit notation for the energy functionals at fixed Φ:

$$\mathcal{E}_L^\Phi(\{t_j\}) = \mathcal{E}_L(\{e^{i\Phi/L}t_j\}) \quad .$$

Here, and in the rest of this section, it is assumed that all t_j are nonnegative. Note that the t_j's now play the role of the $|t_j|$'s.

For any x and y let $d(x,y)$ denote the configuration with $t_j = x$ for j odd and $t_j = y$ for j even, and define the energy density e of a period 2 configuration $d(x,y)$ as in (1.7). Note that e is independent of Φ. In order to remove the degeneracy due to the obvious symmetry under cyclic permutations of the t_j's, we will henceforth adopt the convention that the maximum value of all t's is attained by t_1.

A first ingredient in the proof of Theorem 3 is the following energy estimate, which by itself implies Theorem 3 ii). Let E_L^Φ denote the value of $\mathcal{E}_L^\Phi$ in a minimizing configuration $t_{L,j}^\Phi$. Under the general condition (1.6) ii) on f we can find a constant K, depending only on f, such that $|t_{L,j}^\Phi| \le K$.

9 Lemma. *Assuming only condition ii) on f in* (1.6), *we have for all* $-\pi < \Phi \le \pi$

$$\begin{cases} |E_L^0 - E_L^\Phi| \le 2\Phi^2 K/L & \text{if } L = 2 \bmod 4 \\ \\ |E_L^\pi - E_L^\Phi| \le 2(\pi-\Phi)^2 K/L & \text{if } L = 0 \bmod 4 \end{cases}$$

and

$$\begin{cases} |E_L^\pi - \mathcal{E}_L^\Phi(t_L^0)| \le 4\pi^2 K/L & \text{if } L = 0 \bmod 4 \\ \\ |E_L^\Phi - \mathcal{E}_L^\Phi(t_L^\Psi)| \le 8\pi^2 K/L & \text{for all } \Psi \text{ and all even } L. \end{cases}$$

Because $\mathcal{E}_L^\pi$ attains its minimum E_L^π in a dimerized configuration ($L = 0 \bmod 4$), this lemma implies, for $\Phi = 0$, that even if the true minimum is not dimerized, its energy differs from the best dimerized configuration by $O(1/L)$, which is 2 orders down from $E_L^0 = O(L)$.

Proof : First note that $H(\{t_j\})$ has real matrix elements and therefore has a ground state ψ_L^0 which is *real*, and hence such that $\langle \psi_L^0 \mid c_{j+1,\sigma}^\dagger c_{j,\sigma} \mid \psi_L^0 \rangle$ is also real. Using a gauge transformation that makes $H(\{\exp(i\pi/L)t_j\})$ real one can also see that $H(\{\exp(i\pi/L)t_j\})$ has a ground state ψ_L^π such that

$$\langle \psi_L^\pi \mid c_{j+1,\sigma}^\dagger c_{j,\sigma} \mid \psi_L^\pi \rangle = e^{i\pi/L} R_{j,\sigma} \quad ,$$

with *real* $R_{j,\sigma}$.

Let $\{t_{L,j}^0\}$ be any minimizing configuration of $\mathcal{E}_L^0$, and let ψ_L^0 be a real ground state of $H(\{t_{L,j}^0\})$. Then, by the variational principle,

$$\begin{aligned} E_L^\Phi &\leq \langle \psi_L^0 \mid H(\{\exp(i\Phi/L)t_{L,j}^0\}) \mid \psi_L^0 \rangle + \sum_j f(t_j^0) \\ &= \langle \psi_L^0 \mid H(\{\exp(i\Phi/L)t_{L,j}^0\}) \mid \psi_L^0 \rangle + \sum_j f(t_j^0) \\ &\quad + \sum_{j=1}^L \sum_{\sigma=\uparrow,\downarrow} (e^{i\Phi/L} - 1) t_{L,j}^0 \langle \psi_L^0 \mid c_{j+1,\sigma}^\dagger c_{j,\sigma} \mid \psi_L^0 \rangle + \quad \text{h.c.} \quad . \end{aligned}$$

The sum of the first two terms in the right side of the equality above is E_L^0. Using the reality of ψ_L^0 the last term can be estimated by $4|1 - \cos(\Phi/L)| \sum_j |t_{L,j}^0|$. As $\cos x \geq 1 - x^2/2$, this proves the first estimate of the Lemma. The other inequalities are derived in the same way. **Q.E.D.**

The next lemma is an application of a version of the *Abstract Chessboard Estimate* **[52]** which is given in the Appendix.

10 Lemma. *For any configuration of* $t_j \geq 0$, *with* $d(t_j, t_{j+1})$ *described in* (1.7),

$$\begin{aligned} \frac{1}{L} \sum_{j=1}^L \mathcal{E}_L^0(d(t_j, t_{j+1})) &\leq \mathcal{E}_L^0(\{t_j\}) \quad \text{if } L = 2 \bmod 4 \quad , \\ \frac{1}{L} \sum_{j=1}^L \mathcal{E}_L^\pi(d(t_j, t_{j+1})) &\leq \mathcal{E}_L^\pi(\{t_j\}) \quad \text{if } L = 0 \bmod 4 \quad . \end{aligned} \tag{4.1}$$

Proof : Let $\Phi = 0$ if $L = 2 \bmod 4$ and $\Phi = \pi$ if $L = 0 \bmod 4$. We apply Theorem 15 (with $D = \mathbb{R}^2$) to the following F:

$$F(a_1, \ldots, a_L) = \exp(-\mathcal{E}_L^\Phi(t_1, \ldots, t_L)) \quad ,$$

where $a_j = (t_j, s_j) \in \mathbb{R}^2$. The involution R is defined by $R(t,s) = (s,t)$. The domain $\mathcal{D}$ is taken to be the set of all $(a_1, a_2, \ldots, a_L)$ of the form $((t_1, t_2), (t_2, t_3), \ldots, (t_L, t_1))$. The necessary invariance properties of $\mathcal{D}$ are trivially satisfied. The cylicity of F follows from the invariance of $\mathcal{E}_L^\Phi$ under cyclic permutations of the t_j. The inequality of Lemma 7 translates into Schwarz's inequality for F on $\mathcal{D}$. This becomes obvious with the definitions:

$$\begin{array}{ll} a_1 = (t_1, t_2) & b_1 = (t_L, t_1) \\ a_2 = (t_2, t_3) & b_2 = (t_{L-1}, t_L) \\ \vdots & \vdots \\ a_{L/2} = (t_{L/2}, t_{L/2+1}) & b_{L/2} = (t_{L/2+1}, t_{L/2+2}) \end{array} \quad .$$

Indeed, one then has:

$$\begin{aligned} \exp(-\mathcal{E}_L^\Phi(t_1, \ldots, t_L)) &= F(a_1, a_2, \ldots, a_{L/2}, b_{L/2}, \ldots, b_1) \\ \exp(-\mathcal{E}_L^\Phi(t_1, \ldots, t_{L/2}, t_{L/2+1}, t_{L/2}, \ldots, t_2)) &= F(a_1, a_2, \ldots, a_{L/2}, Ra_{L/2}, \ldots, Ra_1) \\ \exp(-\mathcal{E}_L^\Phi(t_1, t_L, \ldots, t_{L/2+2}, t_{L/2+1}, \ldots, t_L)) &= F(Rb_1, Rb_2, \ldots, Rb_{L/2}, b_{L/2}, \ldots, b_1) \\ \exp(-\mathcal{E}_L^\Phi(t_L, t_{L-1}, \ldots, t_{L/2+1}, t_{L/2+2}, \ldots, t_1)) &= F(b_1, b_2, \ldots, b_{L/2}, Rb_{L/2}, \ldots, Rb_1) \end{aligned}$$

The implication of Theorem 15, in terms of $\mathcal{E}_L^\Phi$ then reads:

$$\mathcal{E}_L^\Phi(t) \geq \frac{1}{L} \sum_{j=1}^{L} \mathcal{E}_L^\Phi(t_j, t_{j+1}, t_j, t_{j+1}, \ldots) \quad ,$$

which is the desired inequality. **Q.E.D.**

11 Lemma. *For the given f let K be a constant such that $|t_{L,j}^\Phi| \leq K$, for all L. For $L = 0 \bmod 4$, let $\{t_{L,j}^0\}$ be any minimizing configuration of $\mathcal{E}_L^0$. Then*

$$|\mathcal{E}_L^\pi(d(t_{L,j}^0, t_{L,j+1}^0)) - E_L^\pi| \leq 4K\pi^2 \quad ,$$

for all $j = 1, 2, \ldots, L$.

Proof : As $L = 0 \bmod 4$ we can apply Lemma 10 to $\mathcal{E}_L^\pi$ and with $t_j = t_{L,j}^0$. We then have

$$\frac{1}{L} \sum_{j=1}^{L} \mathcal{E}_L^\pi(d(t_{L,j}^0, t_{L,j+1})) \leq \mathcal{E}_L^\pi(t_L^0) \quad .$$

By Lemma 9 the right side is bounded by $E_L^\pi + 4\pi^2 K/L$, and hence

$$\frac{1}{L} \sum_{j=1}^{L} \left\{ \mathcal{E}_L^\pi(d(t_{L,j}^0, t_{L,j+1}^0)) - E_L^\pi \right\} \leq \frac{4\pi^2 K}{L} \quad .$$

As each of the terms in the sum is non-negative, the statement of the lemma follows. **Q.E.D.**

12 Lemma. *i) The following limit defines a continuous function e:*

$$\lim_{L \to \infty} \mathcal{E}_L^\Phi(d(x, y)) = e(x, y)$$

The convergence is uniform on compact subsets of $\mathbb{R}^2$.
ii) If e attains its minimum at (x_0, y_0) and (y_0, x_0) and nowhere else, then there exists a sequences $x_L \to x_0$ and $y_L \to y_0$ such that for all $L = 0 \bmod 4$, $d(x_L, y_L)$ is a minimizing

configuration for $\mathcal{E}_L^\pi$, and such that

$$\lim_{L\to\infty} \frac{1}{L}\mathcal{E}_L^\pi(d(x_L,y_L)) = e(x_0,y_0) \quad .$$

Proof : The arguments involved in proving this lemma are fairly standard. We therefore only give a sketch of the proof.

i) We first show that there exists a concave function $\varepsilon(x,y)$, satisfying $\varepsilon(x,y)\le 2|x|+2|y|+|U|$, and such that

$$\varepsilon(x,y) = \lim_{L\to\infty} \frac{1}{L}\lambda_0(H_L(d(x,y))) \quad .$$

For brevity we put $G_L = \lambda_0(H_L(d(x,y)))$. By the variational principle and the fact that $\|c_{j\sigma}\| = 1$ one immediately gets that G_L is "almost subadditive":

$$G_{L_1+L_2} \le G_{L_1} + G_{L_2} + 6(|x|+|y|)$$

and therefore $G_L + 6(|x|+|y|)$ is subadditive. This sequence is also almost monotone:

$$L_1 \ge L_2 \Rightarrow G_{L_1} \le G_{L_2} + \text{Constant}$$

because $G_L \le 0$. It follows that the limit of G_L/L exists and as a limit of concave functions the limit is also concave. The bounds are trivial but they imply continuity and therefore the convergence is uniform on compacts. From Lemma 9 it is obvious that e does not depend on Φ.

ii) From the conditions on f (1.6) one has an apriori bound K on the minimizing t_j: $|t^\pi_{j,L}| \le K$. By Theorem 1, $\mathcal{E}_L^\pi$ always has a dimerized minimizer $d(x_L,y_L)$, and by compactness there always exists a subsequence (x_{L_k},y_{L_k}) converging to (x_*,y_*). By the continuity of e^π and the uniform convergence on compacts

$$\left|\frac{1}{L_k}\mathcal{E}^\pi_{L_k}(d(x_{L_k},y_{L_k})) - e(x_*,y_*)\right| \to 0 \quad .$$

As the $d(x_{L_k},y_{L_k})$ are minimizers it follows that $e(x_*,y_*) = e(x_0,y_0)$ and hence, by assumption, $(x_*,y_*) = (x_0,y_0)$ or $(x_*,y_*) = (y_0,x_0)$. Without loss of generality we can assume $x_0 \ge y_0$. Consider then the new sequence $d(\tilde{x}_L,\tilde{y}_L)$ of minimizers with $(\tilde{x}_L,\tilde{y}_L) = (x_L,y_L)$ or (y_L,x_L), and such that $\tilde{x}_L \ge \tilde{y}_L$ for all L. Then all convergent subsequences $(\tilde{x}_{L_k},\tilde{y}_{L_k})$ of $(\tilde{x}_L,\tilde{y}_L)$ converge to the same limit (x_0,y_0) and hence the sequence is convergent. **Q.E.D.**

Proof of Theorem 3 i):
Let $d(x_L,y_L)$ be a sequence of minimizing configurations for $\mathcal{E}_L^\pi$ and such that x_L and y_L converge to x_0 and y_0 respectively as $L\to\infty$. The existence of such a sequence is guaranteed by Lemma 12.

First we estimate $e(t^0_{L,j},t^0_{L,j+1})$ for a minimizing configuration t^0_L of $\mathcal{E}_L^0$ and any

$j = 1, \ldots, L$.

$$\begin{aligned}
&|e(t^0_{L,j}, t^0_{L,j+1}) - e(x_0, y_0)| \\
&\leq \left| e(t^0_{L,j}, t^0_{L,j+1}) - \frac{1}{L}\mathcal{E}^\pi_L(d(t^0_{L,j}, t^0_{L,j+1})) \right| \\
&\quad + \frac{1}{L}\left| \mathcal{E}^\pi_L(d(t^0_{L,j}, t^0_{L,j+1})) - \mathcal{E}^\pi_L(d(x_L, y_L)) \right| + \frac{1}{L}\left| \mathcal{E}^\pi_L(d(x_L, y_L)) - e(x_0, y_0) \right| \quad .
\end{aligned}$$

All three terms on the right side vanish as $L \to \infty$, uniformly in j: the first term by the uniform convergence on compact sets given by Lemma 12 i), the second by Lemma 11, and the third term by Lemma 12 ii).

The theorem now follows from the uniqueness of the dimerized minimum and compactness. Indeed, suppose one can find arbitrarily large L_k such that

$$|t^0_{L_k,j} - x| + |t^0_{L_k,j+1} - y| \geq \varepsilon \quad \text{and} \quad |t^0_{L_k,j} - y| + |t^0_{L_k,j+1} - x| \geq \varepsilon \quad ,$$

for some $\varepsilon > 0$. By compactness and the continuity of e there would then be a limit point (x', y') of $(t^0_{L_k,j}, t^0_{L_k,j+1})$, for which $e(x', y') = e(x_0, y_0)$. As (x', y') as at least distance ε away from (x_0, y_0) this would imply the existence of another minimizer for e which is ruled out by assumption. **Q.E.D.**

Proof of Theorem 2 :
Let $\Phi = 0$ if $L = 2 \bmod 4$ and $\Phi = \pi$ if $L = 0 \bmod 4$. Denote by $d(x, y)$ the unique dimerized minimizer of $\mathcal{E}^\Phi_L$. Let $\{t^\Phi_j\}$ be any minimzer of $\mathcal{E}^\Phi_L$. As $\mathcal{E}^\Phi_L$ attains its minimum in $\{t^\Phi_L\}$, the inequality of Lemma 10 is an equality for $t_j = t^\Phi_j$. Therefore, all configurations on the left side of (4.1) must be minimizers. These configurations are all dimerized and therefore (by our uniqueness assumption) must all be equal to $d(x, y)$. **Q.E.D.**

5. COUNTEREXAMPLES: RINGS OF LENGTH $L = 0 \bmod 4$ HAVING MINIMIZERS AT ZERO FLUX THAT ARE NOT PERIOD TWO

We will only discuss counterexamples with $U = 0$. It is obvious, then, that counterexamples also exist with small non-vanishing U. However, the presence of a not too large on-site repulsion tends to enhance the dimerization, while nearest neighbour repulsions can reduce it. We have not investigated the effects of interactions on the new instabilities discussed in this section. Our result for the spin-Peierls problem, Theorem 4, which can be interpreted as the $U \to \infty$ limit [**26**], seems to indicate that, when U is very large, the translation symmetry can break down from period one to at most period two. This seems natural because the electrons are more mobile when U is small and, under this condition, other deformations of the lattice can become favorable if the flux is not optimal. We interpret distortions that break the periodicity two as an attempt of the system to mimic the energy lowering effect of a nonvanishing flux. This is also a possible interpretation of the lattice distortions found in two dimensions [**45,46**].

Kennedy and Lieb [**18**] gave an example of a function f (involving a quartic term) which gives rise to a minimum for the model on a square ($L = 4$) which does *not* have periodicity two. Longuet-Higgins and Salem pointed out the possibility of other than period two instabilities a long time ago [**15**], but they expected these to be unimportant and thought the period two instability would always dominate. They only considered the case $L = 2 \bmod 4$ and therefore did not notice that other instabilities can, in fact, occur when $L = 0 \bmod 4$.

Our aim in this section is twofold. First we present a family of functions f that lead to non-period-two minimizers of the zero-flux problem for the ring of eight sites. Then we discuss what instabilities other than period two occur. From the discussion it will become clear how to construct many more examples of non-period-two minima. The properties of the new instabilities, which we study partly only numerically, support our conjectures stated in the introduction.

Counterexample for $L = 8$.

For simplicity we will present just one family of functions f chosen to yield simple values for the minimizing dimerized configuration. It is easy to generalize this example in several directions.

Define a function $f(t)$, for $t \geq 0$, as follows (see Figure 2 for the graph of f.)

$$f(t) = \begin{cases} \frac{1}{10} + \frac{1}{5}(t-1) + \frac{1}{10}(1-t)^2 & \text{if } 0 \leq 4-a \\ \\ \frac{1}{10} + \frac{1}{5}(t-1) + \frac{1}{10}(1-t)^2 + \frac{1}{3a^2}(t-4+a)^3 & \text{if } t \geq 4-a \quad . \end{cases} \tag{5.1}$$

Here a can be any number strictly between 0 and $4 - 5/\sqrt{2} \cong .4645$.

Consider first configurations t_j of the form $t_{2j+1} = x$, $t_{2j} = y$. We always assume $x \geq y \geq 0$. The ground state energy of eight electrons on a ring of eight sites described by the Hamiltonian (1.1) with $U = 0$ is then $4e(x, y)$ where $e(x, y)$ is given by

$$e(x, y) = -x - \sqrt{x^2 + y^2} \quad .$$

For the 8-ring with f given in (5.1), the optimum period two configuration is then determined by the values of $x_0 \geq y_0$ that minimize

$$h(x,y) \equiv e(x,y) + f(x) + f(y) \quad .$$

It is trivial to see that $x_0 > 0$, and as h is differentiable away from $x = 0$ and $h(x,y) \to +\infty$ as x or $y \to +\infty$, (x_0, y_0) must therefore be a critical point of $h(x,y)$ solving the equations

$$\begin{aligned} 1 + \frac{x}{\sqrt{x^2+y^2}} &= f'(x) \\ \frac{y}{\sqrt{x^2+y^2}} &= f'(y) \quad . \end{aligned}$$

A straightforward calculation shows that $(x,y) = (4,3)$ is the unique minimum.

Next we study the stability of the relative minimum (x_0, y_0) under a class of perturbations which break the period two symmetry. For future use we do this for arbitrary $L = 0 \bmod 4$, $L \geq 8$. More specifically we consider configurations of the form $t_{2j+1} = x$, $t_{2j} = y + \varepsilon V_{j+1}$, $j = 1, \ldots, N \bmod N$, with $L = 2N$. As we do not want to introduce a flux, the V_j must be real. One can use analytic perturbation theory to compute the energy as a function of x, y and ε. Up to corrections of $\mathrm{O}(\varepsilon^3)$ one finds

$$\begin{aligned} \text{Kin. Energy } = &- 2\sum_{n=1}^{N} \lambda_n - \varepsilon \hat{V}(0) \sum_{n=1}^{N} \frac{y + x\cos(\alpha n)}{\lambda_n} \\ &+ \varepsilon^2 \sum_{n=1}^{N} \left(\frac{|\hat{V}(0)|^2 (y + x\cos(\alpha n))^2}{\lambda_n^3} - \frac{\sum_{m \neq 2n \bmod N} |\hat{V}(m)|^2}{\lambda_n} \right) - \varepsilon^2 \frac{|\hat{V}(0)|^2}{|x-y|} \\ &- 4\varepsilon^2 \sum_{n,m; \lambda_n \neq \lambda_m} |\hat{V}(n-m)|^2 \frac{P_{n,m}}{\lambda_n(\lambda_n^2 - \lambda_m^2)} \quad , \end{aligned} \tag{5.2}$$

where

$$\lambda_n = \sqrt{x^2 + y^2 + 2xy\cos(\alpha n)}, \quad \alpha = 2\pi/N \quad .$$

and

$$P_{n,m} = y^2 + x^2 \cos(\alpha(n+m)/2))^2 + 2xy\cos(\alpha(n+m)/2)\cos(\alpha(n-m)/2) \quad .$$

$\hat{V}$ is the Fourier transform of V_j: $\hat{V}(q) = (1/N)\sum_j \exp(2\pi i j q/N) V_j$. Note that the coeffient of ε^2 is diagonal in $\hat{V}$. Up to terms $\mathrm{O}(\varepsilon^3)$, the elastic energy is

$$N \left(f(y) + f(x) + \varepsilon f'(y) \sum_j V_j + \tfrac{1}{2}\varepsilon^2 f''(y) \sum_j V_j^2 \right) \quad .$$

In a critical point (x, y) in the set of period two configurations, the terms proportional to ε in the electron energy will cancel the ones in the elastic energy. A perturbation V will then lower the energy for small ε if the total (electron plus elastic energy) coefficient of ε^2 is negative, which means that the optimal dimerized configuration is not the true minimum. Call the coefficient of the ε^2 contribution to the electron energy $-\Delta(x, y)$. Note that this coefficient is always negative. There is an instability whenever

$$\Delta(x_0, y_0) > \frac{N}{2} f''(y_0) \quad . \tag{5.3}$$

We now return to the model on the 8-ring and show that indeed the energy can be lowered by perturbing the dimerized minimum (x_0, y_0) found above. For the 8-ring ($N = 4$) there are four independent perturbations V_i to consider:

$$\begin{aligned} V = (1, 1, 1, 1), \quad V = \sqrt{2}(1, 0, -1, 0) \quad , \\ V = (1, -1, 1, -1), \quad V = \sqrt{2}(0, 1, 0, -1) \quad . \end{aligned}$$

The first, $V = (1, 1, 1, 1)$, respects the period 2 and in the optimum dimerized configuration it cannot lower the energy. The second and the fourth have the same energy because they are translates of each other. We have normalized the V's such that $\sum_i V_i^2 = 4$ (in general we will use the normalization $\sum_i V_i^2 = N$.) Let $-\Delta_0, -\Delta_1, -\Delta_2$ be the coefficients of ε^2 for the first, second and third choice of V respectively. It is convenient to factor out x as a scale factor and to use the ratio $r = y/x$ as the relevant variable, $0 \le r \le 1$. The explicit expressions for the Δ's are:

$$\begin{aligned} x\Delta_0 &= \frac{2}{(1 + r^2)^{3/2}} \\ x\Delta_1 &= 4 - \frac{2}{\sqrt{1 + r^2}} \\ x\Delta_2 &= 2 \quad . \end{aligned}$$

In our example both Δ_1 and Δ_2 satisfy the criterion for instability (5.3):

$$|\Delta_1(4, 3)| = \frac{3}{5} > 2f''(3) = \frac{2}{5}, \qquad |\Delta_2(4, 3)| = \frac{1}{2} > 2f''(3) = \frac{2}{5} \quad .$$

Of course, $\Delta_0(4, 3)$ does not satisfy (5.3), indicating that (4,3) is a stable relative minimum within the set of period two configurations (indeed $\Delta_0(4, 3) = 32/125 < 2/5$). We conclude that for the choice of f defined in (5.1) the energy minimizing configuration of the 8-ring is not period two.

Other than period-two instabilities for arbitrary $L = 0 \bmod 4$.
The behavior of the coefficients of ε^2 in (5.2) for large N gives support to our conjectures 1 and 2 stated in the introduction.

Let $-\Delta_k$ denote the coefficient of ε^2 for $V = V^{(k)}(q)$, where $\hat{V}^{(k)}(q) = (\delta_{q,k}+\delta_{q,N-k})/\sqrt{2}$, $k \neq 0, N/2$, $\hat{V}^{(0)}(q) = \delta_{q,0}$, $\hat{V}^{(N/2)}(q) = \delta_{q,N/2}$. The perturbations are normalized such that their contributions to the elastic energy is identical. Δ_0 and Δ_1 are given by:

$$\Delta_0 = \sum_{n=1}^{N} \frac{x^2 \sin(\alpha n)^2}{\lambda_n^3} \quad ,$$

$$\Delta_1 = \sum_{n=1}^{N} \frac{1}{\lambda_n} + \sum_{n=1}^{N} \left(\frac{1}{\lambda_n} - \frac{1}{\lambda_{n+1}}\right) \frac{P_{n,n+1}}{xy(\cos(\alpha n) - \cos(\alpha(n+1)))} \quad .$$

The stability of a relative minimum (x_0, y_0) within the set of period two configurations requires that $\Delta_0 < (N/2)f''(y_0)$. When $\Delta_0 < (N/2)f''(y_0) < \Delta_1$ such a relative minimum is unstable against the perturbation $\varepsilon V^{(1)}$, which has wavelength $= L$. Numerical investigation of these expressions reveals the following: for $r \equiv y/x < 1$ but close enough to 1 (depending on N), one has $\Delta_1 > \Delta_0$. This is illustrated in Figure 3. Note that the perturbations with $k > 1$ are all stable. We showed in the previous subsection that for $L = 8$ this situation can be realized with a function f satisfying the conditions i and ii) stated in the introduction. It is reasonable to expect that this can be done for all L that are a multiple of 4, but the larger L becomes the more stringent are the restrictions on f. In particular, if one fixes f we expect that for large enough systems the long wavelength instability will not occur and the system will remain in a period two configuration.

A. Appendix

1) Discontinuous and non-convex f

We have assumed throughout this paper that f was a continuous function satisfying some simple conditions as stated in the introduction (1.6). Whether or not f is continuous we can associate a function $\overline{f}$ with f having the following properties: (a) $\overline{f}$ is convex (i.e., $\overline{f}(\lambda t+(1-\lambda)t') \leq \lambda\overline{f}(t)+(1-\lambda)\overline{f}(t')$ for all $0 \leq \lambda \leq 1$ and all $t, t' \geq 0$; (b) $\overline{f}(t) = \sup\{g(t) :$ g is convex and $g(t') \leq f(t')$ for all $t' \geq 0\}$. This function $\overline{f}$ is called the convex hull of f and is automatically continuous for $t > 0$. The following lemma shows that all we really need is that $\overline{f}$ (not f) satisfy conditions i) and ii) of (1.6).

13 Lemma. *Let $\{t_j^\Phi\}$ be a minimizing configuration of $\mathcal{E}_L^\Phi$. Then for all j, $f(t_j^\Phi) = \overline{f}(t_j^\Phi)$, where $\overline{f}$ is the convex hull of f.*

Proof : Let j be arbitrary and fixed. As a function of $t_j = t$ the energy can be written as

$$\begin{aligned}\mathcal{E}(t) &= E(t) + f(t) \\ &= (E(t) + at) + (f(t) - at) = K(t) + g(t) \quad .\end{aligned}$$

We choose $a = (f(t_2) - f(t_1))/(t_2 - t_1)$ where

$$t_1 = \sup\{s < t_j^\Phi \mid f(s) \neq \overline{f}(s)\}, \quad t_2 = \inf\{s > t_j^\Phi \mid f(s) \neq \overline{f}(s)\} \quad .$$

As t appears linearly in the Hamiltonian H, $K(t) = E(t) + at$ is a concave function of t (i.e., $-E(t) - at$ is convex). By construction we also have that $g(t_j^\Phi) \geq g(t_1) = g(t_2)$. Hence, with $0 \leq \alpha \leq 1$ such that $t_j^\Phi = \alpha t_1 + (1-\alpha)t_2$ one has

$$\mathcal{E}(t_j^\Phi) \geq \alpha\mathcal{E}(t_1) + (1-\alpha)\mathcal{E}(t_2)$$

and the inequality is strict if $g(t_j^\Phi) = f(t_j^\Phi) - \overline{f}(t_j^\Phi) \neq 0$. Therefore the minimium can be attained only at t_j where $f(t_j) = \overline{f}(t_j)$. **Q.E.D.**

2) The DLS Lemma for ground states

The following lemma is a ground state version of Lemma 4.1 in [**51**]. An example of this ground state version is given in [**53**]. Note that the matrices A and B need not have real matrix elements. It is obvious how to generalize to reflections that involve an additional unitary transformation. When needed one can in fact apply the lemma as stated below after performing a unitary transformation on one half of the system. In this paper we applied the lemma in two different situations. In the proof of Lemma 5 the two copies of the Hilbert space $\mathcal{H}$ correspond to spin $\uparrow$ and spin $\downarrow$. In Lemma 7 the two spaces refer to the right and left halves of the ring.

14 Lemma. *Let $A, B, C_1, \ldots, C_n$ be a collection of $d \times d$ complex matrices (n could be infinite) with the following properties: A and B are Hermitian (i.e., $A = A^\dagger, B = B^\dagger$), for all i, C_i is real and $\sum_i C_i \otimes C_i$ is symmetric (as a $d^2 \times d^2$ matrix). Let $\lambda_0(A, B)$ denote the lowest eigenvalue of the matrix*

$$T(A,B) \equiv A \otimes \mathbb{I} - \sum_i C_i \otimes C_i + \mathbb{I} \otimes B \quad . \tag{A.1}$$

Then

$$\lambda_0(A,B) \geq \tfrac{1}{2}\left(\lambda_0(A,A^*) + \lambda_0(B^*,B)\right) \quad , \tag{A.2}$$

where A^* denotes the matrix obtained from A by complex conjugation of the matrix elements. In particular

$$\lambda_0(A,B) \geq \min\left(\lambda_0(A,A^*), \lambda_0(B^*,B)\right) \quad .$$

The inequality (A.2) *is strict if for some i*

$$\langle \Omega \mid C_i \otimes \mathbb{I} \mid \Omega \rangle \neq \langle \Omega \mid \mathbb{I} \otimes C_i \mid \Omega \rangle \quad , \tag{A.3}$$

where Ω is any eigenvector for the eigenvalue $\lambda_0(A,B)$ (this is not the only case where the inequality is strict.) In particular all ground states Ω of $T(A,A^*)$ satisfy

$$\langle \Omega \mid C_i \otimes \mathbb{I} \mid \Omega \rangle = \langle \Omega \mid \mathbb{I} \otimes C_i \mid \Omega \rangle \quad .$$

Proof : Let $\{e_j\}$ be a orthonormal basis of $\mathbb{C}^d$ in which the C_i have real matrix elements. Define V to be the antilinear map leaving the e_j invariant: $Ve_j = e_j$. Then $VAV = A^*$ etc. Let Ω be an eigenvector of the smallest eigenvalue of the operator (A.1) and denote by M_{ij} its coefficients in the basis $e_i \otimes e_j$:

$$\Omega = \sum_{i,j} M_{ij} e_i \otimes e_j \quad .$$

We can consider (M_{ij}) as a matrix and use the eigenvectors $\{u_\alpha\}$ of $M^\dagger M$ and $\{v_\alpha\}$ of $MM^\dagger$ to define two new bases:

$$\varphi_\alpha = \sum_j \langle e_j \mid u_\alpha\rangle e_j \quad , \qquad \psi_\alpha = \sum_j \langle e_j \mid v_\alpha\rangle^* e_j \quad .$$

It is then straigthforward to check that

$$\Omega = \sum_\alpha \lambda_\alpha \varphi_\alpha \otimes \psi_\alpha \quad .$$

We can obviously assume that $\lambda_\alpha > 0$ by absorbing a phase in the definition of φ_α and by omitting any vanishing terms in the sum.

Using the fact that $\{\varphi_\alpha\}$ and $\{\psi_\beta\}$ are orthonormal bases the energy of Ω can be expressed as

$$\begin{aligned}\langle \Omega \mid T(A,B) \mid \Omega\rangle = &\sum_\alpha \lambda_\alpha^2 \left(\langle \varphi_\alpha \mid A \mid \varphi_\alpha\rangle + \langle \psi_\alpha \mid B \mid \psi_\alpha\rangle\right) \\ &- \sum_i \sum_{\alpha\beta} \lambda_\alpha\lambda_\beta \langle \varphi_\alpha \mid C_i \mid \varphi_\beta\rangle\langle \psi_\alpha \mid C_i \mid \psi_\beta\rangle \quad .\end{aligned}$$

This energy can directly be compared with the energy of $T(A,A^*)$ and $T(B^*,B)$ in the states Ω_1 and Ω_2 defined by

$$\begin{aligned}\Omega_1 &= \sum_\alpha \lambda_\alpha \varphi_\alpha \otimes V\varphi_\alpha \\ \Omega_2 &= \sum_\alpha \lambda_\alpha V\psi_\alpha \otimes \psi_\alpha\end{aligned}$$

which have the same norm: $\|\Omega\|^2 = \|\Omega_1\|^2 = \|\Omega_2\|^2 = \sum_\alpha \lambda_\alpha^2$. The average of the energies of Ω_1 and Ω_2 is

$$\begin{aligned}&\tfrac{1}{2}(\langle \Omega_1 \mid T(A,A^*) \mid \Omega_1\rangle + \langle \Omega_2 \mid T(B^*,B) \mid \Omega_2\rangle) \\ &= \tfrac{1}{2}\sum_\alpha \lambda_\alpha^2 \left(\langle \varphi_\alpha \mid A \mid \varphi_\alpha\rangle + \langle V\varphi_\alpha \mid A^*V \mid \varphi_\alpha\rangle + \langle V\psi_\alpha \mid B^*V \mid \psi_\alpha\rangle + \langle \psi_\alpha \mid B \mid \psi_\alpha\rangle\right) \\ &- \tfrac{1}{2}\sum_i \sum_{\alpha\beta} \lambda_\alpha\lambda_\beta \left(\langle \varphi_\alpha \mid C_i \mid \varphi_\beta\rangle\langle V\varphi_\alpha \mid C_iV \mid \varphi_\beta\rangle \quad + \langle \psi_\alpha \mid C_i \mid \psi_\beta\rangle\langle V\psi_\alpha \mid C_iV \mid \psi_\beta\rangle\right).\end{aligned} \tag{A.4}$$

Using $\langle V\varphi \mid \psi\rangle = \langle \varphi \mid V^\dagger \mid \psi\rangle^*$, for any two vectors φ, ψ, the hermiticity of A and B and the reality of the C_i, it is straightforward to verify:

$$\begin{aligned}\langle V\varphi_\alpha \mid A^*V \mid \varphi_\alpha\rangle &= \langle \varphi_\alpha \mid A \mid \varphi_\alpha\rangle \\ \langle V\varphi_\alpha \mid C_iV \mid \varphi_\beta\rangle &= \langle \varphi_\alpha \mid C_i \mid \varphi_\beta\rangle^* \quad ,\end{aligned}$$

etc. As $\lambda_\alpha > 0$ we can then apply $2|uv| \leq |u|^2 + |v|^2$ to each term in the double sum of (A.4) to obtain

$$\langle \Omega \mid T(A,B) \mid \Omega\rangle \geq \tfrac{1}{2}\left(\langle \Omega \mid T(A,A^*) \mid \Omega\rangle + \langle \Omega \mid T(B^*,B) \mid \Omega\rangle\right)$$

from which (A.2) directly follows by the variational principle.

The inequality is strict if for some i and some α, β, $\langle \varphi_\alpha \mid C_i \mid \varphi_\beta\rangle \neq \langle \psi_\alpha \mid C_i \mid \psi_\beta\rangle$, for which (A.3) is a sufficient condition. When $A = B^*$, (A.2) is an equality and so

$\langle \varphi_\alpha \mid C_i \mid \varphi_\beta \rangle \neq \langle \psi_\alpha \mid C_i \mid \psi_\beta \rangle$ for all i, α, β in that case. **Q.E.D.**

¿From the proof of the lemma it also follows that any Hamiltonian of the form $T(A, A^*)$, has a ground state Ω satisfying

$$\langle \Omega \mid X \otimes X^* \mid \Omega \rangle \geq 0 \quad .$$

for all observables X on $\mathcal{H}$.

The same state therefore also satisfies

$$\langle \Omega \mid X \otimes \mathbb{1} \mid \Omega \rangle = \langle \Omega \mid \mathbb{1} \otimes X^* \mid \Omega \rangle \quad .$$

In particular if $[X \otimes \mathbb{1}, T(A, A^*)] = 0$, and $X = X^\dagger$, there will be a ground state Ω such that $X \otimes \mathbb{1}\Omega = \mathbb{1} \otimes X^* \Omega = x\Omega$ for some eigenvalue x of X. (This also follows from application of (A.2) with A replaced by $A + c(X - x_1)^2$ and B by $A^* + c(X^* - x_2)^2$, where x_1 and x_2 are the eigenvalues of $X \otimes \mathbb{1}$ and $\mathbb{1} \otimes X^*$ in some ground state of $T(A, A^*)$.

3) The Abstract Chessboard Estimate([**52**])

15 Theorem. *Let D be a set, let $R : D \to D$ be an involution on D ($R^2 =$ identity), and let $F : \mathcal{D} \to \mathbb{C}$ be a complex valued function on a domain $\mathcal{D} \subset D^{\times 2N}$ that has the following invariance properties:*

$$(a_1, \ldots, a_{2N}) \in \mathcal{D} \Rightarrow (a_2, \ldots, a_{2N}, a_1) \in \mathcal{D} \quad ,$$

$$(a_1, \ldots, a_N, b_N, \ldots, b_1) \in \mathcal{D} \Rightarrow (a_1, \ldots, a_N, Ra_N, \ldots, Ra_1), (b_1, \ldots, b_N, Rb_N, \ldots Rb_1) \in \mathcal{D}$$

Assume F obeys

$$F(a_1, \ldots, a_{2N}) = F(a_2, \ldots, a_{2N}, a_1)$$

and

$$|Fa_1, \ldots, a_N, b_N, \ldots, b_1)|^2 \leq F(a_1, \ldots, a_N, Ra_N, \ldots, Ra_1) F(b_1, \ldots, b_N, Rb_N, \ldots, Rb_1) \quad .$$

Then $\|a\| \equiv |F(a, Ra, A, \ldots, Ra)|^{1/2N}$ satisfies

$$|F(a_1, \ldots, a_{2N})| \leq \prod_{j=1}^{2N} \|a_i\| \quad .$$

The proof of the Theorem is exactly the same as in [**52**] Theorem 4.1. In that reference it is also assumed that D is a real vector space and that F is defined on all of D^{2N}. Under these circumstances the inequality of the theorem implies that $\|\cdot\|$ is a seminorm on D, but we do not use this property in this paper.

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We take the opportunity to note three minor technical misstatements in this paper. (A.) The paragraph after eq. (6) is not correct for $N = 2$ because $T_{13} = t_1t_2 + t_3t_4$ and not t_1t_2 in this case. Thus, z has to be replaced by $2z$, but the rest of the argument works. Alternatively, one can compute the eigenvalues of T^2 explicitly since it reduces to a 2×2 matrix. (B.) The uniqueness proof for $N = 2$ needs strengthening. $T^2 = \langle T^2 \rangle$ implies only that $t_1 = t_3$ or $t_2 = t_4$. However, this case can be analyzed explicitly and uniqueness holds. (C.) The statement in *Case 1* that $W(z) \equiv \mathrm{Tr}(2y^2 + z\Omega)^{1/2}$ is an even function of z is correct only when N is even (because the sublattices are then themselves bipartite). However, in all cases $W(z)$ is certainly concave and $dW(z)/dz = (1/2)\,\mathrm{Tr}(2y^2 + z\Omega)^{-1/2}\Omega$, which is zero at $z = 0$. Thus, $W(z)$ is decreasing for $z > 0$ and increasing for $z < 0$, which is what is needed in *Case 1* and *Case 2*.

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FIGURE CAPTIONS

Fig. 1. A ring containing an even number of sites, labeled $1, \ldots, L$. The hopping matrix element t_j is associated with the bond $\{j, j+1\}$. Reflection through the plane indicated by the dashed line interchanges the role of the hoppings labeled $t^{(l)}$ and the ones labeled $t^{(r)}$ (see Lemma 7).

Fig. 2. Graph of the function $f(t)$ defined in (5.1) for $a = .46$. Recall that large t corresponds to small separation w and vice versa.

Fig. 3. Graph of the coefficients $x\Delta_k$ as a function of the ratio $r = y/x$ for $L = 20$ and $k = 0, \ldots, 5$. An instability can occur when $\Delta_k(r) > \Delta_0(r)$. Note that this condition is satisfied only in a small region of r not much smaller than 1, and only for $k = 1$, which corresponds to an instability of wavelength L in real space.