THE LOW-TEMPERATURE LIMIT OF TRANSFER OPERATORS IN FIXED DIMENSION

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Abstract. We construct the 0'th order low-temperature WKB-phase for the first eigenfunction of a transfer operator in a large domain around a non-degenerate critical point for the potential. The 0'th order low-temperature phase is shown to solve the eikonal equation in the strong-coupling limit and we obtain non-local estimates on the 0'th order phase, which are preserved in the limit. We furthermore use the IMS localization technique to study the two highest eigenvalues of the transfer operator in the case where V is allowed to have many non-degenerate global minima.

Part I: Introduction

Section I.1: Short presentation of the results.

This paper is concerned with three problems related to the low-temperature limit of transfer operators. A transfer operator is a bounded positive operator on $L^2(\mathbb{R}^m)$ with integral kernel

$$K(x,y) = (\beta J)^{\frac{m}{2}} e^{-\frac{\beta}{2}V(x)} e^{-\frac{\beta J}{2}|x-y|^2} e^{-\frac{\beta}{2}V(y)},$$

where β is the inverse temperature, J is a coupling constant and $V \in C^\infty(\mathbb{R}^m)$ is a non-negative potential. We will always assume $J > 0$ (ferromagnetism), V has a finite number of non-degenerate global minima (where V equals 0) and $\inf_{|x|>R} V(x) > 0$, for some $R > 0$. One can also consider other dispersion relations than $|x-y|^2$, for example $\omega(x-y)$ where ω is some strictly convex function.

The transfer operator can be viewed as a continuous spin analogue of the transfer matrix, which plays a central role in the study of the Ising model. It was used by

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Helfand and Kac in [HK] to treat the mean-field limit of some discrete spin-systems. The mean-field parameter becomes a ferromagnetic coupling constant for the corresponding transfer operator. See [K] for an exposition. The study undertaken here, by analogy with the Ising model, relates to the statistical mechanics of continuous spin-systems. See [F] and [He5] for details. The relation is sketched for spin-chains in Section III.5.

There are two limits which are of a semiclassical nature. The strong-coupling limit (SC) $J \to +\infty$ and the low-temperature limit (LT) $\beta \to +\infty$. For β or J sufficiently large at least one eigenvalue will appear at the top of the spectrum of K, which can be viewed as the inverse of the spectrum of a Schrödinger operator since

$$K = (2\pi)^{\frac{m}{2}} e^{-\frac{\beta}{2}V} e^{\frac{1}{2\beta J}\Delta} e^{-\frac{\beta}{2}V}.$$

The eigenvalues will be numbered in decreasing order making the first eigenvalue the highest. We furthermore note that, by the Perron-Frobenious Theorem, the first eigenvalue is non-degenerate and its eigenfunction can be chosen strictly positive.

We will in this paper be interested in the following problems

1) A WKB-construction, in large domains, of the first eigenfunction of K in the low-temperature limit.

In [He3] and [He4] Helffer showed how to make WKB-constructions for the first eigenfunction of K in the low-temperature and strong-coupling limits. A semiclassical expansion was obtained for the logarithm of the first eigenfunction and we write $\varphi_0^{(LT)}$ and $\varphi_0^{(SC)}$ for the two 0'th order phases (see Sections I.3 and I.4). The construction of $\varphi_0^{(LT)}$ relied on an application of the local stable manifold Theorem and in this paper we give a more detailed analysis of the problem. We construct $\varphi_0^{(LT)}$ in certain 'large' domains and provide estimates which are of a non-local nature.

2) Study the strong-coupling limit of $\varphi_0^{(LT)}$ and its relation with $\varphi_0^{(SC)}$.

The 0'th order strong-coupling phase $\varphi_0^{(SC)}$ satisfies the eikonal equation

$$|\nabla\varphi|^2 = V,$$

and hence can be described as the generator of the outgoing stable manifold of the Hamiltonian flow generated by $H(x,\xi) = \frac{1}{2}\xi^2 - V(x)$. On the other hand $\varphi_0^{(LT)}$ is the generator of the stable incoming manifold for a discrete dynamical system on phase-space (parametrized by J) and we show that in the strong-coupling limit this dynamical system approximates (when rescaled) the continuous dynamical system given by the Hamiltonian flow of H. This connection enables us to get non-local estimates on solutions to the eikonal equation in 'large' domains as a byproduct of corresponding estimates on the 0'th order low-temperature phase. We note that the eikonal equation enters at leading order in the WKB-analysis of the Schrödinger operator and in semiclassical expansions of Laplace integrals. See [He1], [Sj1] and [Sj2].

The analysis in 1) and 2) can be done in the framework of standard functions (control with respect to dimension), see [Sj2], which will be the topic of future work.

3) Use localizations to study the full transfer operator when V has many non-degenerate global minima.

We use an IMS type localiztion technique, which is similar (but simpler) to the one employed in [Si] to analyze the first two eigenvalues of the Schrödinger operator in the semiclassical limit. We determine the logarithm of the first eigenvalue, using the expansion coming from the WKB-analysis, up to an $O(h^\infty)$ error. As for the splitting between the two first eigenvalues we consider two cases. For a symmetric double well potential we show that the splitting vanishes exponentially in the low-temperature limit. In the case of a unique global minimum we show that, up to an exponentially small error, the splitting is given by the splitting of the localized problem, which can be treated by harmonic approximation (see [He5]).

Section I.2: Overview and acknowledgements.

The paper is divided into three parts. The present part is an introduction, which is primarily concerned with an exposition of the WKB-construction for the highest eigenvalue of the transfer operator in the low-temperature and strong-coupling limits, and the corresponding eigenfunctions. In Section I.3 the crucial step of determining the low-temperature WKB-phase to 0'th order is explained and in Section I.4 the corresponding step for the strong-coupling limit is recalled. A relation between these two limits is exploited in Section I.5 to indicate how one can obtain solutions to the eikonal equation as limits of 0'th order low-temperature phases. In particular we get global solutions if the potential is globally convex.

Part II of the paper is concerned with the construction of the WKB-phases based on the characterizations derived in Part I. In Section II.1 we construct the 0'th order low-temperature phase and provide bounds on its Hessian. In Section II.2 we construct a Hamiltonian flow which we use in Section II.3 to obtain solutions to the eikonal equation following the idea outlined in Section I.5. We give some extra results on the 0'th order low-temperature phase and the solution to the eikonal equation in Section II.4.

The last part of the paper connects the expansion obtained in Part II with the problem of determining the first eigenvalue of the transfer operator. In Section III.1 we show that the restriction of the transfer operators to neighbourhoods of local minima of the potential contain all the low-temperature information. In Section III.2 we prove that the first eigenvalue of the restricted tranfer operator is correctly described by the WKB-construction and we analyze the second eigenvalue in the case of a unique global minimum. In Section III.3 we comment on global constructions in the case where the potential is globally convex. In III.4 we discuss the consequences of the results for classical spin-chains and we compare with the recent results of [BJS].

The references to work related to WKB-constructions for Schrödinger operators are chosen based on relevance to control with respect to dimension and are not intended to represent the subject as a whole.

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Section I.3: The low-temperature limit.

Throughout the paper we will for the sake of brevity use the notation f' for ∇f, the gradient of f. In the case where f depends on more than one variable we will write $(\nabla_x f)(x, y)$ in order to avoid confusion. The same notation will be used for Hessians.

In the introduction we simplify the exposition by assuming that the potential $V \in C^\infty(\mathbb{R}^m)$ is globally convex $V'' > 0$ and has a unique global minimum at 0

$$V(0) = V'(0) = 0.$$

We define the transfer operator K by its kernel

$$K(x, y) = (\pi h)^{-\frac{m}{2}} e^{-\frac{1}{2h}V(x)} e^{-\frac{J}{2h}|x-y|^2} e^{-\frac{1}{2h}V(y)}.$$

Notice that we have replaced the inverse temperature by a semiclassical parameter $h = \beta^{-1}$ and chosen a more natural prefactor for the limit considered.

In order to iteratively construct semiclassical expansions for the first eigenvalue of the transfer operator in the low-temperature limit we make the following ansatz for the first eigenfunction

$$\psi_1(x; h) = e^{-\frac{1}{h}\varphi(x;h)}, \qquad \varphi(x; h) \sim \sum_{k=0}^{\infty} \varphi_k(x) h^k, \tag{3.1}$$

where $\sim$ will denote formal expansions. This type of ansatz was used for Schrödinger operators in [Sj1] instead of the more traditional ansatz, $\psi_1 = a e^{-\frac{1}{h}\varphi_0}$, where the amplitude a is a formal power series in h. The reason is that the control of terms with respect to dimension is difficult with the latter approach.

As for the eigenvalue we suppose

$$\lambda_1(h) = e^{-F(h)}, \qquad F(h) \sim \sum_{k=0}^{\infty} F_k h^k. \tag{3.2}$$

The idea is to determine φ and F inductively by requiring that the integral below is equal to 1 or rather $e^{O(h^\infty)}$.

$$e^{F(h)} \int_{\mathbb{R}^m} e^{\frac{1}{h}\varphi(x;h)} K(x,y) e^{-\frac{1}{h}\varphi(y;h)} dy. \tag{3.3}$$

The strategy is to make a coordinate transformation to bring the integrand into a certain form depending on the scaling of h. We consider a change of coordinates $y \to \xi(y;x,h)$, where ξ has a formal expansion, which gives the integral (3.3) above the form

$$(\pi h)^{-\frac{m}{2}} \int_{\mathbb{R}^m} e^{-\frac{1}{h}\xi^2(y;x,h) + \ln\det \nabla_y \xi(y;x,h)} dy. \tag{3.4}$$

This will imply that $F(h)$ is formally an expansion of the logarithm of the first eigenvalue. We make the further assumption that ξ is the gradient with respect to y of a function, in order to make its derivative symmetric. That is we look for

$$\xi(y;x,h) = \nabla_y f(x,y;h), \qquad f(x,y;h) \sim \sum_{k=0}^{\infty} f_k(x,y) h^k. \tag{3.5}$$

To ensure that the determinant of the Hessian of f is positive (at any finite order) for small h we make the assumption that f_0, the coordinate change to first order, is a convex function of y for any x. Using the explicit form of the integral kernel of the transfer operator we find the equation between formal power series

$$\begin{aligned}\varphi(y;h) - \varphi(x;h) + \frac{1}{2}(V(x) + V(y)) + \frac{J}{2}|x-y|^2 \\ = |\nabla_y f(x,y;h)|^2 - h \ln\det \nabla_y^2 f(x,y;h) + hF(h).\end{aligned} \tag{3.6}$$

Consider the 0'th order equation

$$\varphi_0(y) - \varphi_0(x) + \frac{1}{2}(V(x) + V(y)) + \frac{J}{2}|x-y|^2 = |\nabla_y f_0(x,y)|^2. \tag{3.7}$$

Notice that we have to determine the two unknowns φ_0 and f_0 at the same time. Fix $\varphi_0(0) = 0$ (can be chosen freely). By the assumption that f_0 is convex in y for any x we find that for any x there exists a unique critical point $\Phi_J(x)$ at which $\nabla_y f_0$ vanishes. Note that the gradient of the right hand side with respect to both x and y vanishes at the critical manifold $(x, \Phi_J(x))$. This gives the following equations (for $\Phi_J(x)$)

$$\begin{aligned}\varphi_0'(y) + \frac{1}{2}V'(y) + J(y-x) = 0 \\ -\varphi'(x) + \frac{1}{2}V'(x) + J(x-y) = 0.\end{aligned} \tag{3.8}$$

Notice that given $(x, \varphi_0'(x))$ we can determine $(\Phi_J(x), \varphi_0(\Phi_J(x)))$. Inspired by this observation we introduce a diffeomorphism of the symplectic space $\mathbb{R}^m_x \times \mathbb{R}^m_\xi$

$$\kappa(x, \xi; J) = (\kappa_x(x, \xi; J), \kappa_\xi(x, \xi; J)) = (y, \eta),$$

given by the set of equations

$$\begin{aligned} \eta + \frac{1}{2}V'(y) + J(y - x) &= 0 \\ -\xi + \frac{1}{2}V'(x) + J(x - y) &= 0. \end{aligned} \tag{3.9}$$

The 0'th order phase φ_0 will now by (3.8) satisfy the relation

$$\kappa(x, \varphi_0'(x); J) = (\Phi_J(x), \varphi_0'(\Phi_J(x))). \tag{3.10}$$

In other words the graph of φ_0' is a stable manifold for the fixed point $(0, 0)$ of the discrete dynamical system κ. One can see by convexity that the critical point $\Phi_J(x)$ will be closer to 0 than x (if φ_0 is convex) which indicates that the graph is the incoming manifold. One can check that $(0, 0)$ is a hyperbolic fixed point and that κ is a symplectic transformation which implies that the stable manifolds are Lagrangian submanifolds of $\mathbb{R}^{2m}$.

From (3.7) one can also see that the 0'th order phase will be a fixed point of the transformation

$$\tilde{T}\varphi(x) = \frac{1}{2}V(x) + \inf_{y \in \mathbb{R}^m}(\frac{1}{2}V(y) + \varphi(y) + \frac{J}{2}|x - y|^2), \tag{3.11}$$

which turns out to be a contraction on convex functions. This observation will be the key to the global construction given in Section II.1. Notice that the stable manifold Theorem always gives a local construction. This approach was taken in [He3] and in [He4] control with respect to dimension is achieved. Iterating the transformation in (3.11) starting with the function $\varphi = \frac{1}{2}V$ gives a pointwisely non-decreasing sequence which is bounded from above. Hence it converges to some function which is locally Lipschitz. This is true for any positive potential but we lack explicit control of the limit. See [He2], [He3] or [He5].

Section I.4: The strong-coupling limit.

This limit has been treated by Helffer in [He4] and by Helffer and Ramond in [HeRa] and we present here the results. The semiclassical parameter will be

$$h = J^{-\frac{1}{2}}.$$

We put $\beta = 1$ (or alternatively transform it into the potential).

One can proceed here as in the previous section and look for a suitable change of coordinates. The scaling is however different and one should aim at bringing the integral (3.3) on the form

$$(\pi h^2)^{-\frac{m}{2}} \int_{\mathbb{R}^m} e^{-\frac{1}{h^2}|\xi(y;x,h)|^2 + \ln\det \nabla_y \xi(y;x,h)} dy$$

instead of the form (3.4). (Notice that the transfer operator in this limit has an extra factor of $h^{-\frac{m}{2}}$.) This will give the equation (between formal power series)

$$\begin{aligned} h\varphi(y;h) - h\varphi(x;h) + \frac{h^2}{2}(V(x)+V(y)) + \frac{J}{2}|x-y|^2 \\ = |\nabla_y f(x,y;h)|^2 - h^2 \ln\det \nabla_y^2 f(x,y;h) + h^2 F(h). \qquad (4.1) \end{aligned}$$

Analyzing this one finds that the 0'th order WKB-Phase φ_0 must satisfy the eikonal equation

$$|\varphi_0'(x)|^2 = 2V(x). \qquad (4.2)$$

One can also describe φ_0 in way more parallel to what was done in the previous section. Notice that $(x, \varphi_0'(x))$ lies on the zero-energy manifold for the Hamiltonian

$$H(x,\xi) = \frac{1}{2}\xi^2 - V(x). \qquad (4.3)$$

In fact $(x, \varphi_0'(x))$ will be the outgoing stable manifold at the hyperbolic fixed point $(0,0)$ for the continuous symplectic dynamical system given by the Hamiltonian flow $\Psi_t(x,\xi)$ for the Hamiltonian above

$$\begin{aligned} \dot{\Psi}_t(x,\xi) &= (\nabla_\xi H)(\Psi_t(x,\xi)) \\ \dot{\Psi}_t(x,\xi) &= -(\nabla_x H)(\Psi_t(x,\xi)) \\ \Psi_0(x,\xi) &= (x,\xi). \qquad (4.4) \end{aligned}$$

Section I.5: A connection between the two limits.

In this section we will explain a central point of this paper which links the low-temperature limit with the strong-coupling limit. Suppose we take the low-temperature limit and then subsequently ask what happens when the coupling becomes large. We can on a formal level think of this as replacing J by the semi-classical parameter h^{-2} which was chosen to be β^2. The scaling is now h^{-1} on the potential and h^{-3} on the coupling term. If one tries to construct a 0'th order phase with this scaling one finds exactly as in the previous section that it must satisfy the eikonal equation and that it enters as a h^{-2} term. Now the 0'th order low-temperature phase depends on J and entered on the h^{-1} level. In order to get the scaling h^{-2} it is natural to suggest that $J^{-\frac{1}{2}}\varphi_0^{(LT)}$ should scale as a constant for large coupling constants J. In fact it not only scales as a constant it converges to the strong-coupling 0'th order phase. In other words

$$\lim_{J\to\infty} J^{-\frac{1}{2}}\varphi_0^{(LT)} = \varphi_0^{(SC)}.$$

One can also see this connection more clearly by taking a second look at the discrete dynamical system (3.9). In order to clarify this we make a symplectic scaling tranformation of κ to get a new dynamical system

$$\tau(x,\xi;J) = (\kappa_x(x, J^{\frac{1}{2}}\xi;J), J^{-\frac{1}{2}}\kappa_\xi(x, J^{\frac{1}{2}}\xi;J)). \tag{5.1}$$

This system then have its incoming manifold described by the graph of $J^{-\frac{1}{2}}\varphi_0'^{(LT)}$ and $\tau = (\tau_x, \tau_\xi)$ can be written using the Taylor expansion as

$$\tau(x,\xi;J) = \begin{pmatrix} x \\ \xi \end{pmatrix} - J^{-\frac{1}{2}}\begin{pmatrix} \xi \\ V'(x) \end{pmatrix} + \frac{1}{2}J^{-1}\begin{pmatrix} V'(x) \\ V''(x)\xi \end{pmatrix} + J^{-\frac{3}{2}}\begin{pmatrix} 0 \\ r_J(x,\xi) \end{pmatrix}, \tag{5.2}$$

where the remainder

$$r_J(x,\xi) = \frac{1}{4}V''(x)V'(x) + \frac{1}{4}\int_0^1 \langle \nabla^3 V(z_t), (\xi - \frac{1}{2}J^{-\frac{1}{2}}V'(x)) \otimes (\xi - \frac{1}{2}J^{-\frac{1}{2}}V'(x))\rangle dt$$

and $z_t = tx + (1-t)(x-\tau_x)$. The remainder is clearly bounded uniformly in large J. Applying τ once, in the limit of large J, corresponds to taking an infinitesimal step along the Hamiltonian flow (4.4) for the Hamiltonian (4.3) and in fact by iterating τ one recovers the Euler-Cauchy method (up to the remainder term) for integrating the differential equation (4.4). Thus it is no miracle that one can obtain the strong-coupling phase from the low-temperature phase and we will in fact adopt some ideas from theoretical numerical analysis to achieve this end (see [D]).

This seems to be a new way of constructing solutions to the eikonal equation in a non-local way. Notice that the proof of the local stable manifold Theorem for continuous dynamical system goes through the discrete case (see [I]) and in some sense this is also what is done here. What is more important is probably that as a byproduct we can get non-local estimates on solutions to the eikonal equation as strong-coupling limits of corresponding estimates on the 0'th order low-temperature phase, which in some sense is easier to handle.

Section I.6: Higher order phases.

In this section we return to the equations (3.6) and (4.1) and obtain equations for higher order phases (in the low-temperature limit). See [He4] for a more complete exposition. From the discussion in Sections 3 and 4 we know how to produce 0'th order phases.

First of all we get an equation for the coordinate change to 0'th order now that we now the 0'th order phase (see (3.7))

$$|\nabla_y f_0(x,y)|^2 = W_x(y) = \varphi_0(y) - \varphi_0(x) + \frac{1}{2}(V(y)+V(x)) + \frac{J}{2}|x-y|^2. \tag{6.1}$$

This is an eikonal equation for a convex potential with critical point at $y = \Phi_J(x)$ and it can be solved (globally) using the connection with the 0'th order phase in the strong-coupling limit. Here x enters as a parameter in the potential W_x.

Before we proceed we need a lemma which appeared in [Sj1], [He1], [He4] and [HeRa]. It is used to determine which terms of $\ln\det\nabla_y^2 f(x,y;h)$ one should use at a given order.

Lemma I.6.1. *Let $h \to M(h)$ be a smooth family of positive $m\times m$ matrices with an asymptotic expansion $M(h) \sim \sum_{k\geq 0} M_k h^k$ and suppose $M_0 > 0$. Then $L(h) = \ln\det M(h)$ has an asymptotic expansion $L(h) \sim \sum_{k\geq 0} L_k h^k$ where*

$$L_0 = \ln\det M_0$$

and for $k \geq 1$

$$L_k = \sum_{n=1}^{k} \sum_{\substack{j_1,\dots,j_n\geq 1\\ j_1+\cdots+j_n=k}} (-1)^{n-1}(n-1)!\,\mathrm{tr}\{\Pi_{i=1}^n M_0^{-1}M_{j_i}\}.$$

As for the 1'st order phase we get

$$\varphi_1(y) - \varphi_1(x) = 2\nabla_y f_0(x,y)\cdot\nabla_y f_1(x,y) - \ln\det\nabla_y^2 f_0(x,y) + F_0. \tag{6.2}$$

Considering this equation along the critical manifold $y = \Phi_J(x)$ gives

$$\varphi_1(x) = \varphi_1(\Phi_J(x)) + \ln\det\nabla_y^2 f_0(x,\Phi_J(x)) - F_0. \tag{6.3}$$

The idea is to choose

$$F_0 = \ln\det\nabla_y^2 f_0(0,0)$$

as the eigenvalue to 0'th order and then iterate keeping in mind that $\Phi_J^{(k)}(x) \to 0$ as $k\to\infty$. Subtracting the constant part of $\ln\det(\nabla_y^2 f_0)(x,\Phi_J(x))$ will ensure convergence. In order to control the regularity of this construction we will need to have good estimates of iterates of Φ_J and its derivatives.

The coordinate change to 1'st order satisfies a standard transport equation

$$2\nabla_y f_1(x,y)\cdot\nabla f_0(x,y) = \varphi_1(y) - \varphi_1(x) + \ln\det\nabla_y^2 f_0(x,y) - F_0 \tag{6.4}$$

which can be solved explicitly around $y = \Phi_J(x)$. In particular it can be solved in the same domains for which we construct the 0'th order coordinate change. (See for example [He1], [He4] or [Sj1]). The rest of the way is simply a repetition of the procedure described for the 1'st order phase and coordinate change. First set the eigenvalue at k'th order equal to the known term in the k'th order equation, obtained from (3.6), evaluated at $(0,0)$ and iterate towards $(0,0)$ along the critical manifold to obtain the k'th order phase. Finally solve the corresponding transport equation and obtain the coordinate change to k'th order.

Part II: Constructing the 0'th order phases

Section II.1: A family of discrete dynamical systems.

In this section we construct the 0'th order WKB-phase in the low-temperature limit.

Let $V \in C^\infty(\mathbb{R}^m)$ have a non-degenerate local minimum at $x = 0$ with $V(0) = 0$. Suppose V is convex in a neigbourhood of 0 and define

$$\Omega = \{x \in \mathbb{R}^m : V''(x) > 0\}.$$

Let $D_\infty \subset \Omega$ be an open set containing 0 and let $d \in C^\infty(D_\infty)$ be a smooth non-negative convex function with $d(0) = d'(0) = 0$.

For $R > 0$ we consider the sets

$$D_R = d^{-1}([0, R]).$$

By assumption D_R is convex and closed for small R but this need not be the case for large R unless for example $\Omega = \mathbb{R}^m$. Let

$$R_0 = \sup\{R > 0 : D_R \text{ is convex and closed, and } V'(x) \cdot d'(x) > 0, x \in D_R \backslash \{0\}\}. \tag{1.1}$$

We can choose d such that $R_0 = R_0(d) > 0$ since both $d = V_{|\Omega}$ and $d = x^2_{|\Omega}$ are valid choices. For $R < R_0$ the boundary of D_R is a level set for d

$$\partial D_R = d^{-1}(\{R\}).$$

We redefine for notational simplicity

$$D_\infty = \overset{\circ}{D}_{R_0}.$$

We will consider the family of discrete dynamical systems on $\mathbb{R}^m \times \mathbb{R}^m$ introduced in (I.3.9). It has the form

$$\begin{aligned}\kappa(x,\xi;J) &= (\kappa_x(x,\xi;J), \kappa_\xi(x,\xi;J)) \\ &= \begin{pmatrix} x - J^{-1}\xi + J^{-1}\frac{1}{2}V'(x) \\ \xi - \frac{1}{2}J^{-1}(V'(\kappa_x(x,\xi;J)) - V'(x)) \end{pmatrix}. \end{aligned} \tag{1.2}$$

The aim is to construct a branch of the incoming manifold near the hyperbolic fixed point $(0,0)$, more precisely in the open convex set D_∞, as the graph of the gradient of a function which is a fixed point for the following operation on convex functions on D_∞ (see (I.3.11))

$$[\tilde{T}\varphi](x) = \frac{1}{2}V(x) + \inf_{y\in D_\infty}(\frac{1}{2}V(y) + \varphi(y) + \frac{J}{2}|x-y|^2).$$

This is closely connected with the Legendre transform in the sense that

$$[\tilde{T}\varphi](x) = \frac{1}{2}V(x) + \frac{J}{2}x^2 - [L(\frac{1}{2}V + \varphi + \frac{J}{2}y^2)](Jx),$$

where

$$[L\psi](x) = \sup_{y\in D_\infty}(x\cdot y - \psi(y))$$

is the Legendre transform of ψ. Consider now a class of functions

$$\tilde{\mathcal{S}} = \{\varphi \in C^\infty(D_\infty) : \varphi(0) = 0, \varphi'' \geq 0 \quad \text{and} \quad \varphi'\cdot d' \geq 0\}.$$

We wish to show that $\tilde{\mathcal{S}}$ is invariant under the transformation above. Obviously $[\tilde{T}\varphi](0) = 0$.

The first assertion is that the infimum is attained in D_∞. For $x \in D_\infty$ we consider $z \in \partial D_{d(x)}$ and $t \geq 0$. Compute for $z_t = z - td'(z) \in D_{d(x)}$

$$\begin{aligned}&\frac{d}{dt}(\frac{1}{2}V(z_t) + \varphi(z_t) + \frac{J}{2}|z_t - x|^2)_{|t=0} \\ &\qquad = -(\frac{1}{2}V'(z) + \varphi'(z) + J(z-x))\cdot d'(z).\end{aligned}$$

Since $x \in D_{d(x)}$, $D_{d(x)}$ is convex and $d'(z)$ is normal to $\partial D_{d(x)}$ at z, we find that $(z-x)\cdot d'(z)$ is positive. By this argument, and the assumption that $V'(z)\cdot d'(z) > 0$, we conclude that the infimum, $\Phi(x)$, is attained at a point in the interior of $D_{d(x)} \subset D_\infty$. In particular this implies that Φ satisfies the critical equation

$$J(x - \Phi(x)) = \frac{1}{2}V'(\Phi(x)) + \varphi'(\Phi(x)) \tag{1.3}$$

and the inequality

$$d(\Phi(x)) < d(x), \quad \text{for} \quad x \neq 0. \tag{1.4}$$

Using that $\Phi(x)$ is also the critical point for the Legendre transform, we see that Φ is smooth. We can now compute

$$[\tilde{T}\varphi]'(x) = \frac{1}{2}V'(x) + J(x - \Phi(x)). \tag{1.5}$$

Using (1.4), and the convexity argument again, we find that $[\tilde{T}\varphi]'(x) \cdot d'(x) \geq 0$, for $x \in D_\infty$. Hence $\tilde{\mathcal{S}}$ is invariant under $\tilde{T}$.

Since Φ only depends on φ', we obtain a new fixed point problem on the following space of vector valued functions with symmetric derivatives

$$\mathcal{S} = \{\xi \in C^\infty(D_\infty; \mathbb{R}^m) : \xi(0) = 0, \xi' \geq 0, \quad \text{and} \quad \xi \cdot d' \geq 0\}. \tag{1.6}$$

Notice that elements of $\mathcal{S}$ are gradients of convex functions (from $\tilde{\mathcal{S}}$). The operation is (see (1.3) and (1.5))

$$[T\xi](x) = \frac{1}{2}V'(x) + J(x - \Phi(x)), \quad \text{where} \quad J(x - \Phi(x)) = \frac{1}{2}V'(\Phi(x)) + \xi(\Phi(x)). \tag{1.7}$$

Taking the derivative of these relations we find that

$$\Phi' = J(J + \frac{1}{2}V''(\Phi) + \xi'(\Phi))^{-1} \tag{1.8}$$

and

$$[T\xi]' = \frac{1}{2}V'' + J(\frac{1}{2}V''(\Phi) + \xi'(\Phi))(J + \frac{1}{2}V''(\Phi) + \xi'(\Phi))^{-1}. \tag{1.9}$$

This shows that functions ξ with non-negative derivative are mapped into functions $T\xi$ with positive derivative. Hence T maps gradients of convex functions into gradients of convex functions. We also see by (1.8) that Φ's derivative is positive.

We define

$$\begin{aligned} \lambda_l(x) &= \sup\{v : V''(y) \geq vI \quad \text{for} \quad y \in D_{d(x)}\} \\ \lambda_u(x) &= \inf\{v : V''(y) \leq vI \quad \text{for} \quad y \in D_{d(x)}\} \end{aligned} \tag{1.10}$$

We will now show that the map T has a unique fixed point in $\mathcal{S}$. Let $\xi_1, \xi_2 \in \mathcal{S}$ and write Φ_1 and Φ_2 for the corresponding vector-fields. By (1.7) and Taylor's formula

$$T\xi_1 - T\xi_2 = J(\Phi_2 - \Phi_1)$$

and

$$\begin{aligned} J(\Phi_2 - \Phi_1) &= \frac{1}{2}(V'(\Phi_1) - V'(\Phi_2)) + \xi_1(\Phi_1) - \xi_2(\Phi_2) \\ &= \int_0^1 \{\frac{1}{2}V''(x_t) + \xi_1'(x_t)\}dt(\Phi_1 - \Phi_2) + \xi_1(\Phi_2) - \xi_2(\Phi_2), \end{aligned}$$

where (by (1.4)) $x_t = t\Phi_1(x) + (1-t)\Phi_2(x) \in D_{d(x)}$. This shows that

$$J|\Phi_1 - \Phi_2|^2 \le -\frac{1}{2}\lambda_l(x)|\Phi_1 - \Phi_2|^2 + |\xi_1(\Phi_2) - \xi_2(\Phi_2)||\Phi_1 - \Phi_2| \tag{1.11}$$

and hence we have the following inequality for any $0 < R < R_0$

$$\sup_{x \in \overset{\circ}{D}_R} |(T\xi_1)(x) - (T\xi_2)(x)| \le \frac{J}{J + \frac{1}{2}\inf_{x \in D_R} \lambda_l(x)} \sup_{x \in \overset{\circ}{D}_R} |\xi_1(x) - \xi_2(x)|.$$

This shows that T restricted to functions on $\overset{\circ}{D}_R$ is a strict contraction, with respect to the supremums norm, and hence has a fixed point in the closure of $\mathcal{S}$ (with $R_0 = R$). Obviously choosing R larger provides an extension of the fixed point to a larger domain and hence the fixed point extends to an L^∞_{loc} function on D_∞. We will write ξ_J for this fixed point.

Theorem II.1.1. *The set $\mathcal{S}$ is invariant under the transformation T and there exists a unique fixed point $\xi_J \in \mathcal{S}$ whose graph is the local incoming manifold in D_∞ for the symplectomorphism κ at the hyperbolic fixed point $(0,0)$. The function φ_0 defined by $\varphi_0(0) = 0$ and $\varphi_0' = \xi_J$ is the 0'th order low-temperature phase and it satisfies the estimate*

$$a_l(x)I \le \varphi_0''(x) \le a_u(x)I, \quad x \in D_\infty, \tag{1.12}$$

where

$$a_l(x) = \sqrt{J\lambda_l(x) + \frac{1}{4}\lambda_l(x)^2} \quad \textit{and} \quad a_u(x) = \sqrt{J\lambda_u(x) + \frac{1}{4}\lambda_u(x)^2}. \tag{1.13}$$

Proof. For $\xi \in \mathcal{S}$ we define

$$\sigma_l^\xi(x) = \sup\{\lambda \ge 0 : \xi'(y) \ge \lambda I, y \in D_{d(x)}\}$$
$$\sigma_u^\xi(x) = \inf\{\lambda \ge 0 : \xi'(y) \le \lambda I, y \in D_{d(x)}\}.$$

By (1.8-9) we have the a priori bounds

$$J(J + \frac{1}{2}\lambda_u + \sigma_u^\xi)^{-1} I \le \Phi' \le J(J + \frac{1}{2}\lambda_l + \sigma_l^\xi)^{-1} I \tag{1.14}$$

and

$$\frac{1}{2}\lambda_l + \frac{J(\frac{1}{2}\lambda_l + \sigma_l^\xi)}{J + \frac{1}{2}\lambda_l + \sigma_l^\xi} \le [T\xi]' \le \frac{1}{2}\lambda_u + \frac{J(\frac{1}{2}\lambda_u + \sigma_u^\xi)}{J + \frac{1}{2}\lambda_u + \sigma_u^\xi}. \tag{1.15}$$

This leads us to investigate the (contraction) map $\rho_t : [0,\infty) \to [0,\infty)$, given by

$$\rho_t(s) = \frac{1}{2}t + \frac{J(\frac{1}{2}t + s)}{J + \frac{1}{2}t + s},$$

for $t > 0$. Solving the equation $\rho_t(s) = s$ we find the fixed point

$$s_f(t) = \sqrt{Jt + \frac{1}{4}t^2}.$$

The estimate (1.15) now implies that the set

$$\mathcal{S}_{a_l,a_u} = \{\xi \in \mathcal{S} : a_l(x)I \le \xi'(x) \le a_u(x)I, x \in D_\infty\} \tag{1.16}$$

is invariant under T and since

$$a_l(0)x \in \mathcal{S}_{a_l,a_u},$$

we find that it is a non-empty subset of $\mathcal{S}$. Hence the fixed point ξ_J restricted to $\overset{\circ}{D}_R$ lies in the closure of $\mathcal{S}_{a_l,a_u}$ and is in particular a global Lipschitz function.

Pick a sequence $\{\eta_n\} \subset \mathcal{S}_{a_l,a_u}$ such that $\eta_n \to \xi_J$. Then the corresponding sequence of vector-fields Ψ_n is Cauchy by (1.11) (with respect to the supremum norm on $\overset{\circ}{D}_R$) and we write Φ_J for the limit which is also Lipschitz and satisfies the critical equation in (1.7) with ξ_J. This implies since ξ_J is a fixed point for T

$$\kappa(x, \xi_J(x); J) = (\Phi_J(x), \xi_J(\Phi_J(x))). \tag{1.17}$$

We now estimate using (1.14)

$$|\Phi_J| = \lim_{n\to\infty} |\Psi_n| \le \frac{J}{J + \frac{1}{2}\lambda_l}|x|, \tag{1.18}$$

which in turn imply that (recall $\xi_J(0) = 0$)

$$\kappa^{(k)}(x, \xi_J(x); J) \to (0,0), \quad \text{for} \quad k \to +\infty.$$

This shows, together with (1.17), that the graph of ξ_J is contained in the stable incoming manifold for κ at the fixed point (0,0). From the global stable manifold Theorem, see [I], we know that the incoming manifold has dimension m and the same regularity as V'. This implies that ξ_J is smooth and its graph, over $\overset{\circ}{D}_R$, coincides with the local incoming manifold for κ. Since $0 < R < R_0$ was arbitrary we find $\xi_J \in \mathcal{S}$.

The 0'th order phase is now chosen as prescribed which is possible since ξ_J' is symmetric. $\square$

Let $\xi \in \mathcal{S}_{a_l,a_u}$ and write Φ for the corresponding vector-field. From (1.12) and (1.14) we get the estimates

$$J(J+\frac{1}{2}\lambda_u+a_u)^{-1}I \leq \Phi' \leq J(J+\frac{1}{2}\lambda_l+a_l)^{-1}I, \tag{1.19}$$

which imply the following improvement of the a priori estimate (1.18)

$$|\Phi(x)| \leq \frac{J}{J+\frac{1}{2}\lambda_l(x)+a_l(x)}|x|. \tag{1.20}$$

Notice that the graph of $-\xi_J$ is the local outgoing manifold. We remark that the global incoming manifold can have several layers in D_∞ and the global outgoing and incoming manifolds might even coincide. See the monograph [I] for the theory of stable manifolds for hyperbolic fixed points.

Section II.2: Approximating the Hamiltonian system.

We saw in the last section, as discussed in Section I.5, that the incoming manifolds for κ scale as $J^{-\frac{1}{2}}$. We therefore consider the symplectically scaled transformation τ introduced in (I.5.1). This symplectomorphism again has $(0,0)$ as a hyperbolic fixed point and the graph of $J^{-\frac{1}{2}}\xi_J$ is the local incoming manifold for $(0,0)$ in D_∞.

In this section we will prove that τ, in the limit $J\to\infty$, gives the Hamiltonian flow (I.4.4) for the Hamiltonian (I.4.3). Here V will be any smooth function on $\mathbb{R}^m$. The ideas employed here are common in theoretical numerical analysis, see for example [D].

We introduce a family of diffeomorphisms

$$\Psi_t^n(x,\xi) = \tau^{(n)}(x,\xi;\frac{n^2}{t^2}), \quad t<0, \tag{2.1}$$

and put $\Psi_0^n(x,\xi)=(x,\xi)$. Obviously $\Psi_t^n(x,\xi)$ is continuous at $t=0$.

Let $\mathcal{P} \subset \mathbb{R}_x^m \times \mathbb{R}_\xi^m \times \mathbb{R}_t$ be the set of (x,ξ,t) for which the Hamiltonian flow (I.4.4) starting at (x,ξ) can be extended to time t. If V'' is globally bounded the system is globally Lipschitz and $\mathcal{P} = \mathbb{R}_x^m \times \mathbb{R}_\xi^m \times \mathbb{R}_t$. If V grows too rapidly the flow can move of to infinity in finite time.

For $t\in\mathbb{R}$ we define

$$\tilde{\tau}(x,\xi;t,n) = \begin{pmatrix} x \\ \xi \end{pmatrix} - \frac{t}{n}\begin{pmatrix} \xi \\ V'(x) \end{pmatrix} + \frac{t^2}{2n^2}\begin{pmatrix} V'(x) \\ V''(x)\xi \end{pmatrix} \tag{2.2}$$

and

$$\tilde{\Psi}_t^n(x,\xi) = \tilde{\tau}^{(n)}(x,\xi;t,n). \tag{2.3}$$

Then we have

Theorem II.2.1. *Let $V \in C^\infty(\mathbb{R}^m)$. The diffeomorphisms $\tilde{\Psi}^n_t$ converges to the Hamiltonian flow (I.4.4), for the Hamiltonian (I.4.3), locally uniformly in $\mathcal{P}$. In particular for any compact $K \subset \mathcal{P}$ there exists $C_K > 0$ such that*

$$\sup_{(x,\xi,t)\in K} |\tilde{\Psi}^n_t(x,\xi) - \Psi_t(x,\xi)| \leq C_K n^{-2}.$$

Proof. Let $K \subset \mathcal{P}$ be compact. We can assume that if $(x,\xi,t) \in K$, $t \geq 0$ ($t \leq 0$), then $(\psi_{t-s}(x,\xi), r) \in K$ for $0 \leq r \leq s \leq t$ ($0 \geq r \geq s \geq t$).

Using Taylor's formula on the Hamiltonian flow around $t = 0$ we find

$$\Psi_t(x,\xi) = \begin{pmatrix} x \\ \xi \end{pmatrix} - t \begin{pmatrix} \xi \\ V'(x) \end{pmatrix} + \frac{t^2}{2} \begin{pmatrix} V'(x) \\ V''(x)\xi \end{pmatrix} + t^3 R_t(x,\xi),$$

where the remainder $R_t(x,\xi)$ is bounded uniformly in K. By this computation we easily conclude that the error after one iteration is

$$\sup_{(x,\xi,t)\in K} |\Psi_{\frac{t}{n}}(x,\xi) - \tilde{\tau}(x,\xi;t,n)| \leq C_0 n^{-3}.$$

The next step will be to estimate how much $\tilde{\tau}$ distorts phase-space. We compute for (x,ξ) and (y,η) in $\mathbb{R}^m \times \mathbb{R}^m$. Using (I.5.2) and (2.2) we find the estimate

$$|\tilde{\tau}(x,\xi;t,n) - \tilde{\tau}(y,\eta;t,n)| \leq \left(1 + \frac{C_1}{n}\right) \left| \begin{pmatrix} x \\ \xi \end{pmatrix} - \begin{pmatrix} y \\ \eta \end{pmatrix} \right| + \frac{C_2}{n^3}, \qquad (2.4)$$

where the constants can be chosen locally uniformly in (x,ξ,y,η,t) and $n \geq 1$. Pick C_1 and C_2 such that the estimate holds uniformly in (x,ξ,y,η,t,n) with $(x,\xi,t) \in K$, $(y,\eta,t) \in K$ and $n \geq 1$.

We can now make the estimate

$$\begin{aligned} |\Psi_t(x,\xi) - \tilde{\Psi}^n_t(x,\xi)| &\leq |\Psi_t(x,\xi) - \tilde{\tau}(\Psi_{t-\frac{t}{n}}(x,\xi);t,n)| \\ &\quad + |\tilde{\tau}(\Psi_{t-\frac{t}{n}}(x,\xi);t,n) - \tilde{\tau}^{(n)}(x,\xi;t,n)| \\ &\leq \left(1 + \frac{C_1}{n}\right) |\Psi_{t-\frac{t}{n}}(x,\xi) - \tilde{\tau}^{(n-1)}(x,\xi;t,n)| + \frac{C_0 + C_2}{n^3}. \end{aligned}$$

Iterating this estimate using the choice of C_1 and C_2 and the inequality

$$\left(1 + \frac{C_1}{n}\right)^k \leq \left(1 + \frac{C_1}{n}\right)^n, \quad \text{for} \quad 0 \leq k \leq n,$$

gives

$$|\Psi_t(x,\xi) - \tilde{\Psi}^n_t(x,\xi)| \leq \frac{C_0 + C_2}{n^2} \left(1 + \frac{C_1}{n}\right)^n. \qquad (2.5)$$

Since $(1 + \frac{C_1}{n})^n \to e^{C_1}$ as $n \to \infty$, we conclude the result. $\square$

Let

$$\mathcal{P}_- = \{(x,\xi,t) \in \mathcal{P} : t \leq 0\}.$$

Then we have

Corollary II.2.2. *The family of diffeomorphisms Ψ_t^n, $t \leq 0$ converges to the Hamiltonian flow (I.4.4), for the Hamiltonian (I.4.3), locally uniformly in $\mathcal{P}_-$. In particular for any compact $K \subset \mathcal{P}_-$ there exists $C_K > 0$ such that*

$$\sup_{(x,\xi,t)\in K} |\Psi_t(x,\xi) - \Psi_t^n(x,\xi)| \leq C_K n^{-2}.$$

Section II.3: Solving the eikonal equation.

In this section we return to the potentials considered in Section II.1 and the family of fixed points $\eta_J = J^{-\frac{1}{2}}\xi_J$ connected to the rescaled diffeomorphism τ (see (I.5.1)). We know that

$$b_l(x)I \leq \eta_J'(x) \leq b_u(x)I,$$

where

$$b_l(x) = J^{-\frac{1}{2}}a_l(x) \quad \text{and} \quad b_u(x) = J^{-\frac{1}{2}}a_u(x).$$

Consider an $0 < R < R_0$. Since the derivative of η_J is bounded from above and below uniformly in $J \geq 1$ and $x \in D_R$ we find that the sequence $\eta_J(x)$ is uniformly bounded for $x \in \mathcal{D}_R$ and $J \geq 1$. We pick a compact set $\Sigma_R \subset \mathbb{R}^m$ such that

$$(x, \eta_J(x)) \in D_R \times \Sigma_R, \quad \text{for} \quad x \in D_R \quad \text{and} \quad J \geq 1.$$

In the following x will be a point in D_R and $\xi \in \Sigma_R$ an accumulation point for $\eta_J(x)$. We pick a sequence $\{J_k\}$ (with $1 \leq J_k \to \infty$) such that $\eta_{J_k}(x) \to \xi$ for $k \to \infty$.

Lemma II.3.1. *Let $t \leq 0$ and $\epsilon > 0$. There exist $N_0 > 0$ and $C > 0$ such that*

$$|\Psi_t^n(x,\eta) - \Psi_t^n(x,\eta')| < \epsilon + C|\eta - \eta'|$$

uniformly in $n \geq N_0$ and $\eta, \eta' \in \Sigma_R$.

Proof. We estimate as for (2.4)

$$\begin{aligned} &|\tau(x,\eta;\frac{n^2}{t^2}) - \tau(y,\eta';\frac{n^2}{t^2})| \\ &\qquad \leq \left(1 + \frac{C_1|t|}{n} + \frac{C_2t^2}{n^2}\right)\left|\begin{pmatrix} x \\ \eta \end{pmatrix} - \begin{pmatrix} y \\ \eta' \end{pmatrix}\right| + \frac{C_3|t|^3}{n^3}, \end{aligned}$$

where the constants are chosen uniformly in $D_R \times \Sigma_R$. By iterating this estimate we get (see the argument for (2.5))

$$|\Psi_t^n(x,\eta) - \Psi_t^n(x,\eta')| \leq \left(1 + \frac{C_1|t|}{n} + \frac{C_2t^2}{n^2}\right)^n \left\{\frac{C_3|t|^3}{n^2} + |\eta - \eta'|\right\}$$

and the lemma follows. □

The following lemma is the first example of a statement which is proved by choosing invariant subsets of $\mathcal{S}_{a_l,a_u}$ (see (1.16)) thereby implying statements for the fixed point. This idea will be central for the next section.

Lemma II.3.2. *The map $J \to \eta_J$ is smooth and we have the following bound for all $0 < R < R_0$ and $J \geq 1$*

$$\sup_{x \in D_R} |\frac{d}{dJ}\eta_J(x)| \leq C_R J^{-1},$$

for some (non-decreasing family) $C_R > 0$.

Proof. That ξ_J (and hence η_J) is smooth with respect to $J > 0$ follows from the stable manifold Theorem, see [I]. It can be verified independently however by applying the idea of this proof to higher order derivatives in J. This means that T can be viewed as a map on the set $\mathcal{S}^1 = C^\infty((0,\infty); \mathcal{S}_{a_l,a_u})$ and it has a unique fixed point ξ_J.

In analogy with the proof of Theorem 1.1 we write for $\xi \in \mathcal{S}^1$ with associated vector-field Φ

$$\sigma_\xi(J; x) = \sup_{y \in D_{d(x)}} |\frac{d}{dJ}\xi(J; y)|.$$

Taking the derivative with respect to J of the critical relation in (1.7), we get

$$\frac{d}{dJ}\Phi = J^{-1}\Phi'(x - \Phi - \frac{d}{dJ}\xi(\Phi; J)).$$

This implies

$$\frac{d}{dJ}T\xi = (I - \Phi')(x - \Phi) + \Phi'\frac{d}{dJ}\xi(\Phi; J)$$

which together with (1.4), (1.8) and (1.20) gives the estimate

$$\sigma_{T\xi}(J; x) \leq t_J(x) + \theta(x)\sigma_\xi(J; x),$$

where

$$\theta = \frac{J}{J + \frac{1}{2}\lambda_l + a_l}$$

and

$$t_J(x) = \left(\frac{\frac{1}{2}\lambda_u(x) + a_u(x)}{J + \frac{1}{2}\lambda_u(x) + a_u(x)}\right)^2 \sup_{y \in D_{d(x)}} \|y\|.$$

As in the proof of Theorem 1.1, we can consider the (contraction) map $\rho_{t,\theta}(s) = t + \theta s$ and conclude that the fixed point ξ_J must satisfy the estimate $\sigma_{\xi_J} \leq s_f(t_J, \theta)$, where

$$s_f(t_J, \theta) = \frac{t_J}{1 - \theta}$$

is the fixed point of $\rho_{t_J,\theta}$.

Note that for J large we have by (1.13)

$$t_J \sim J^{-1}\lambda_u \sup_{y\in D_{d(x)}} \|y\| \quad \text{and} \quad 1-\theta \sim J^{-\frac{1}{2}}\sqrt{\lambda_l}$$

uniformly in D_R, $0 < R < R_0$. The result now follows since $\eta_J = J^{-\frac{1}{2}}\xi_J$. $\square$

We now combine the first two lemmas to get control of the Hamiltonian flow for $t < 0$.

Lemma II.3.3. *The Hamiltonian flow beginning at (x, ξ) can be extended to $t = -\infty$. Furthermore*

$$\Psi_t(x,\xi) \in D_{d(x)} \times \Sigma_{d(x)}, \quad \textit{for} \quad t \leq 0.$$

Proof. Assume the Hamiltonian flow exists for $0 \geq t > t_c > -\infty$. Let $\epsilon > 0$. By Corollary 2.2 there exists $N_1 > 0$ such that

$$|\Psi_t(x,\xi) - \Psi_t^n(x,\xi)| \leq \frac{\epsilon}{3},$$

for $n \geq N_1$. By Lemma 3.1, applied with $(\eta,\eta') = (\xi, \eta_{J_k})$, we thus get an N_0 and a K_0 such that

$$|\Psi_t(x,\xi) - \Psi_t^n(x,\eta_{J_k}(x))| \leq \frac{2\epsilon}{3}, \tag{3.1}$$

for $n \geq \max\{N_0, N_1\}$ and $k \geq K_0$.

Let $\tilde{J}_k = \frac{([t\sqrt{J_k}]+1)^2}{t^2}$, $t < 0$. Then $n_{k,t} = t\sqrt{\tilde{J}_k}$ is an integer and

$$0 \leq \tilde{J}_k - J_k \leq \frac{4}{t^2}(1 + t\sqrt{J_k}).$$

Using Lemma 3.2 we thus get (uniformly in k and $D_{d(x)}$)

$$\begin{aligned} |\eta_{J_k} - \eta_{\tilde{J}_k}| &\leq \int_{\tilde{J}_k}^{J_k} |\frac{d}{dJ}\eta_J| dJ \\ &\leq C\frac{1+t\sqrt{J_k}}{t^2 J_k}. \end{aligned}$$

This estimate shows, in conjunction with (3.1), that for each $0 > t > t_c$ there exists $K_0 > 0$ large enough such that

$$|\Psi_t(x,\xi) - \Psi_t^{n_{k,t}}(x,\eta_{\tilde{J}_k}(x))| \leq \epsilon,$$

for $k \geq K_0$. Here we have used Lemma 3.1 with $(\eta,\eta') = (\eta_{J_k}, \eta_{\tilde{J}_k})$.

This implies that $\Psi_t(x,\xi)$ can be approximated by elements of $D_{d(x)} \times \Sigma_{d(x)}$, see (1.17). Since this set is closed, $\Psi_t(x,\xi)$ must be there itself. We have now shown

$$\Psi_t(x,\xi) \in D_{d(x)} \times \Sigma_{d(x)}, \quad \text{for} \quad 0 \geq t > t_c.$$

The flow is thus contained in a compact set and we find by general theory that it can be extended beyond t_c, see [HiSm]. This concludes the proof. $\square$

Corollary II.3.4. *The accumulation point (x, ξ) lies on the outgoing manifold for the hyperbolic fixed point $(0, 0)$ of the Hamiltonian flow.*

Proof. Let $x \in D_\infty \backslash \{0\}$. We write $(x(t), \xi(t))$ for the flow $\Psi_t(x, \xi)$ with $\Psi_0(x, \xi) = (x, \xi)$. Suppose there exist $\epsilon > 0$ and a sequence $\{t_n\}_{n \in \mathbb{N}}$ with $t_n \to -\infty$ such that

$$x(t_n)^2 + \xi(t_n)^2 \geq \epsilon.$$

First notice that by Hamiltons equations (I.4.4) and convexity of V the quantities

$$h_1(t) = x(t) \cdot \xi(t) \quad \text{and} \quad h_2(t) = \xi(t) \cdot V'(x(t))$$

are increasing in t (and positive at $t = 0$).

Now compute for $t, t_0 < 0$

$$\begin{aligned} x(t)^2 + \xi(t)^2 &= \int_{t_0}^{t} \int_{t_0}^{s} \frac{d}{dr}(h_1(r) + h_2(r)) dr ds \\ &\quad + (t - t_0)(h_1(t_0) + h_2(t_0)) + x(t_0)^2 + \xi(t_0)^2 \\ &\geq -|t_0 - t|(h_1(0) + h_2(0)) + x(t_0)^2 + \xi(t_0)^2. \end{aligned}$$

This shows that for $\delta = \frac{\epsilon}{2(h_1(0)+h_2(0))}$ we have

$$x^2(t) + \xi^2(t) \geq \frac{\epsilon}{2} \quad \text{for} \quad |t_n - t| \leq \delta, n \in \mathbb{N}.$$

In particular this implies the bound (for $\rho = \min\{1, \lambda_l(x)\}$)

$$\begin{aligned} h_1(t_n) &= -\int_{t_n}^{0} \xi(s)^2 + x(s) \cdot V'(x(s)) ds + h_1(0) \\ &\leq -\rho \int_{t_n}^{0} x(s)^2 + \xi(s)^2 ds + h_1(0) \\ &\leq -n\rho\epsilon\delta + h_1(0), \end{aligned}$$

which contradicts the requirement given by Lemma 3.3 that the trajectory stays in the compact set $D_{d(x)} \times \Sigma_{d(x)}$. □

This result shows that the gradient of the 0'th order low-temperature phase φ_0 converges to the gradient of a solution to the eikonal equation. More precisely

Theorem II.3.5. *Let φ_0 be as in Theorem II.1.1. The limit*

$$\lim_{J \to \infty} J^{-\frac{1}{2}} \varphi_0 = \psi$$

exists and is attained locally uniformly in D_∞. The function ψ is a smooth non-negative convex function with $\psi(0) = 0$ and it satisfies the eikonal equation (I.4.2) in D_∞. We furthermore have the bounds

$$\sqrt{\lambda_l(x)}I \le \psi''(x) \le \sqrt{\lambda_u(x)}I, \quad \textit{for} \quad x \in D_\infty.$$

Proof. As mentioned earlier the outgoing manifold may have many branches in $D_\infty \times \mathbb{R}^m$. We will argue that there is at most one point $(x, \xi) \in D_\infty \times \mathbb{R}^m$ on the outgoing manifold which propagated by Ψ_t does not leave this set on its way to $(0, 0)$.

If this is the case then Corollary 3.4 shows that for each x such a $\xi = \eta_\infty(x)$ exists and since it is unique it is the limit of $\eta_J(x)$ as $J \to \infty$ and hence Lipschitz. Since the outgoing manifold of the Hamiltonian flow is m dimensional and smooth we conclude that η_∞ is smooth and the branch of the outgoing manifold in $D_\infty \times \mathbb{R}^m$ going through $(0, 0)$ is the graph of η_∞. The function ψ in the theorem is chosen such that $\psi' = \eta_\infty$, which is possible since η'_∞ is symmetric. That ψ solves the eikonal equation follows from conservation of energy.

Let $x \in D_\infty$ and suppose there exists $\xi_1, \xi_2 \in \mathbb{R}^m$ such that $\Psi_{-t}(x, \xi_1) = (x_1(-t), \xi_1(-t))$ and $\Psi_{-t}(x, \xi_2) = (x_2(-t), \xi_2(-t))$ stays in $D_{d(x)} \times \mathbb{R}^m$ and converges to $(0, 0)$ as $t \to +\infty$. Let $h(t) = (x_1(-t) - x_2(-t)) \cdot (\xi_1(-t) - \xi_2(-t))$. We have

$$\dot{h}(t) = -|\xi_1(-t) - \xi_2(-t)|^2 - (x_1(-t) - x_2(-1)) \cdot (V'(x_1(-t)) - V'(x_2(-t))). \quad (3.4)$$

Since $x_1(-t), x_2(-t) \in D_{d(x)}$ and V is convex on the convex set $D_{d(x)}$ with Hessian bounded from below, we find by Taylor's formula

$$\dot{h}(t) \le -|\xi_1(-t) - \xi_2(-t)|^2 - \rho|x_1(-t) - x_2(-t)|^2,$$

for some $\rho > 0$.

This shows on one hand that $h(t)$ is non-increasing as $t \to +\infty$. On the other hand we know that $h(0) = 0$ and

$$\lim_{t \to \infty} h(t) = 0$$

by assumption. Hence $h(t) = 0$ for any $t \ge 0$. Since the right-hand side of (3.4) is now forced to vanish for all $t \ge 0$, we have in particular that $\xi_1 = \xi_2$. This concludes the proof. $\square$

We note that the estimates provided by a_l and a_u are not optimal since they are required to be monotone, see (1.10). Only in the case where V is of quadratic type do they even capture the growthrate. Around the minimum however these bounds are optimal.

Section II.4: Further results for the 0'th order phases.

In this section we discuss some additional properties of the constructions presented in Part II. The first observation concerns symmetries. Let $G \subset O(m)$ be a subgroup of the orthogonal group. We say a function $f : \mathbb{R}^m \to \mathbb{R}$ is G-invariant if

$$f(gx) = f(x), \quad \text{for} \quad g \in G.$$

Notice that if $\tilde{d}$ is a comparison function for a G-invariant potential V then

$$d(x) = \int_G \tilde{d}(gx)dg$$

is a G-invariant comparison function for V. Here dg is the Haar measure on G. Now let d be G-invariant (then $gD_R = D_R$, for $g \in G$). The following result follows by replacing $\tilde{\mathcal{S}}$ and $\mathcal{S}$ in Section 1 by

$$\tilde{\mathcal{S}}_G = \{\varphi \in \tilde{\mathcal{S}} : \varphi(gx) = \varphi(x), g \in G, x \in D_\infty\}$$

and

$$\mathcal{S}_G = \{\xi \in \mathcal{S} : g^{-1}\xi(gx) = \xi(x), g \in G, x \in D_\infty\},$$

noting that the construction using functions from these classes is invariant under G.

Proposition II.4.1. *Let G be a subgroup of $O(m)$ and suppose V is G-invariant. Then the low-temperature phase constructed in Theorem II.1.1 and the solution to the eikonal equation given by Theorem II.3.5 are G-invariant.*

The next observation is concerned with extending the domain for which we have a solution. Let $\mathcal{D} = \mathcal{D}(V)$ denote the class of comparison functions, d, for a potential V in the sense of Section 1. For each d we have a maximal convex domain $D_\infty(d)$ in which the construction works. Pathching these domains together we get solutions in domains of the form

$$\cup_{d\in\mathcal{D}} D_\infty(d). \tag{4.1}$$

This can be used in applications to get solutions in some non-convex domains and we will use it in a later paper to construct solutions in l^∞ neighbourhoods of the critical point with control in high dimension. See [Sj1] and [He4]. In [So] local solutions to the eikonal equation are constructed in l^2 balls with radius scaling like the square root of the dimension.

Let $d \geq 0$ be a smooth convex function on an open subset of $\mathbb{R}^m$ containing zero. Let $D_\infty = \overset{\circ}{D}_R$ for some $R > 0$ for which D_∞ is convex. For such R and $\sigma > 0$ we consider the potential class

$$\mathcal{V}_{R,\sigma} = \{V \in C^\infty(D_\infty) : V \geq 0, V(0) = 0, V'' \geq \sigma I, V' \cdot d' > 0 \text{ in } D_\infty\backslash\{0\}\}.$$

Write

$$\theta(\sigma) = \frac{J}{J + \frac{1}{2}\sigma + \sqrt{J\sigma + \frac{1}{4}\sigma^2}}.$$

Proposition II.4.2. *Let $V_1, V_2 \in \mathcal{V}_{R,\sigma}$. We have*

$$\sup_{x\in D_\infty} \|\nabla(\varphi_{0,1} - \varphi_{0,2})\| \leq \frac{1}{2(1-\theta(\sigma))} \sup_{x\in D_\infty} \|\nabla(V_1 - V_2)\|,$$

and for the associated vector-fields, see (1.7), we have

$$\sup_{x\in D_\infty} \|\Phi_1 - \Phi_2\| \leq \frac{\theta(\sigma)+1}{2J(1-\theta(\sigma))} \sup_{x\in D_\infty} \|\nabla(V_1 - V_2)\|.$$

As for the solutions to the eikonal equation ψ_1 and ψ_2 we have

$$\sup_{x\in D_\infty} \|\nabla(\psi_1 - \psi_2)\| \leq \frac{1}{2\sqrt{\sigma}} \sup_{x\in D_\infty} \|\nabla(V_1 - V_2)\|.$$

Proof. Write

$$\mathcal{S}_\sigma = \{\xi \in \mathcal{S} : \xi' \geq \sqrt{J\sigma + \frac{1}{4}\sigma^2 I}\}.$$

Then $\mathcal{S}_\sigma$ is invariant under T_1 and T_2 by the choice of $\mathcal{V}_{R,\sigma}$ and the proof of the lower bound in Theorem 1.1. Here T_i will denote the map T associated with the potential V_i.

Let $\xi_1, \xi_2 \in \mathcal{S}_\sigma$ and write Φ_1 and Φ_2 for the vector-fields obtained from ξ_1 and ξ_2 using the critical equation in (1.7) with potentials V_1 and V_2 respectively. We compute as for the argument which gave the contraction property of T on $\mathcal{S}$, see (1.11), and get for $\xi_1, \xi_2 \in \mathcal{S}_\sigma$.

$$\sup_{x\in D_\infty} \|\Phi_1 - \Phi_2\| \leq \frac{\theta(\sigma)}{J} \sup_{x\in D_\infty} \|\xi_1 - \xi_2\|.$$

Choosing ξ_1 and ξ_2 as the fixed points of T_1 and T_2 restricted to $\mathcal{S}_\sigma$ thus imply

$$\sup_{x\in D_\infty} \|\xi_1 - \xi_2\| \leq \frac{1}{2(1-\theta(\sigma))} \sup_{x\in D_\infty} \|\nabla(V_1 - V_2)\|.$$

This gives the first estimate since $\nabla\varphi_{0,i} = \xi_i$.

The second estimate now follows directly from the first and the last follows from Theorem 3.5 by noting that

$$\lim_{J\to\infty} J^{-\frac{1}{2}} \frac{1}{2(1-\theta(\sigma))} = \frac{1}{2\sqrt{\sigma}}.$$

$\square$

This proposition is a special case of a more general result for parameter dependent potentials V_z which gives continuity of mixed derivatives of the low-temperature phase with respect to the potential, provided the potentials are taken from some a priori class (like $\mathcal{V}_{R,\sigma}$). We do not elaborate further but refer the reader to a coming paper in which we will control the constructions presented here with respect to the dimension m using the framework of standard function calculus (see [Sj2]).

Part III: Global analysis

Section III.1: Restriction to global minima.

In this part of the paper we wish to analyze the localization properties of the transfer operator in the low-temperature limit and use the WKB-construction of Helffer, as presented in Sections I.3 and I.6, of the localized first eigenfunction to gain information on the corresponding eigenvalue. We note that the methods presented here does not directly extend to give control with respect to high dimension.

Let $V \in C^\infty(\mathbb{R}^m)$ be a non-negative potential with a finite number of non-degenerate global minima, $\{z_1, \ldots, z_k\}$, with $V(z_i) = 0$. Choose R small enough such that V is convex in each of the k disjoint balls

$$B_i = B(z_i, R) = \{x \in \mathbb{R}^m : |x - z_i| \leq R\}.$$

Write $B_0 = \mathbb{R}^m \setminus \cup_{i=1}^k B_i$ and assume

$$\rho = \inf_{x \in B_0} V(x) > 0.$$

We write

$$r_0 = \min_{1 \leq i < j \leq k} \operatorname{dist}(B_i, B_j).$$

Let K_i, $1 \leq i \leq k$, be the restriction of the full transfer operator K (see Section I.3) to the ball B_i. That is the bounded operator with the kernel

$$K_i(x, y) = K(x, y)_{|B_i \times B_i}$$

on the Hilbert space $L^2(B_i)$. One can verify that K becomes trace class if V satisfies some growth estimate at infinity (see [He5]). These properties are however not needed for the analysis here.

Let χ_i be the characteristic function for the ball B_i, $0 \leq i \leq k$. First we estimate the contribution from the region away from the global minima

$$\|\chi_0 K\| \leq \sup_{x \in B_0} e^{-\frac{1}{2h} V(x)} = e^{-\frac{\rho}{2h}}. \tag{1.1}$$

Let $\varphi_1, \varphi_2 \in L^2(\mathbb{R}^m)$. For $1 \le i < j \le k$ we have

$$\begin{aligned}|\langle \chi_i \varphi_1, K\chi_j \varphi_2\rangle| &\le (\pi h)^{-\frac{m}{2}} \int_{\mathbb{R}^m}\int_{\mathbb{R}^m} \chi_i(x)\chi_j(y) e^{-\frac{J}{2h}|x-y|^2} |\varphi_1(x)||\varphi_2(y)| dx dy \\ &\le (\pi h)^{-\frac{m}{2}} |B| e^{-\frac{J r_0^2}{2h}} \|\varphi_1\|\|\varphi_2\|,\end{aligned}$$

where $|B|$ denotes the volume of the balls B_i. This implies the following estimate on the coupling between minima

$$\|\chi_i K \chi_j\| \le (\pi h)^{-\frac{m}{2}} e^{-\frac{J r_0^2}{2h}} \quad \text{for} \quad 1 \le i < j \le k. \tag{1.2}$$

In the following C will denote positive constants and δ will denote positive exponents. Both C and δ may vary within the same calculation but are uniform with respect to small $h > 0$.

We choose the first eigenfunction ψ_1 normalized and positive and we write λ_1^i, $1 \le i \le k$, for the first eigenvalue of the operator K_i. Let

$$\mu_1 = \max_{1 \le i \le k} \lambda_1^i.$$

The estimates (1.1-2) show on one hand that

$$\begin{aligned}\lambda_1 &\le \sum_{i=1}^k \langle \chi_i \psi_1, K \chi_i \psi_1\rangle + Ce^{-\frac{\delta}{h}} \\ &\le \sum_{i=1}^k \lambda_1^i \|\chi_i \psi_1\|^2 + Ce^{-\frac{\delta}{h}} \\ &\le \mu_1 + Ce^{-\frac{\delta}{h}}.\end{aligned} \tag{1.3}$$

On the other hand we write ψ_1^i for the normalized first eigenfunction of the operator K_i extended to the whole space by the 0 function. Again we choose it positive. Then by the variational principle

$$\begin{aligned}\lambda_1 &\ge \max_{1 \le i \le k} \langle \psi_1^i, K \psi_1^i\rangle \\ &= \max_{1 \le i \le k} \langle \psi_1^i, K_i \psi_1^i\rangle \\ &= \mu_1.\end{aligned} \tag{1.4}$$

We have the a priori estimate (see [He2] and [He5])

$$0 < C_1 \le \lambda_1 \le C_2, \tag{1.5}$$

where C_1 and C_2 can be chosen uniformly in small $h > 0$. The lower bound follows from an application of Segal's Lemma (or harmonic approximation which also applies to the μ_1^i's). The estimates (1.3-5) give

Theorem III.1.1. *There exists $h_0 > 0$ such that*

$$\mu_1 \leq \lambda_1 \leq \mu_1(1 + Ce^{-\frac{\delta}{h}})$$

for $0 < h \leq h_0$.

The estimates (1.1-2) also yields

Proposition III.1.2. *Let V be a symmetric double well. (i.e. $z_1 = -z_2$ and $V(x) = V(-x)$.) There exists $h_0 > 0$ such that*

$$0 \leq \ln \frac{\lambda_1}{\lambda_2} \leq Ce^{-\frac{\delta}{h}},$$

for $0 < h \leq h_0$.

Proof. Choose $B_2 = -B_1$ disjoint and let

$$\tilde{\psi}_2 = \chi_1 \psi_1 - \chi_2 \psi_1.$$

Then by symmetry $\tilde{\psi_2} \perp \psi_1$ and by (1.1) and (1.5)

$$\begin{aligned} 1 \geq \|\tilde{\psi}_2\|^2 &= 1 - \|\chi_0 \psi_1\|^2 \\ &= 1 - \lambda_1^{-1} \|\chi_0 K \psi_1\|^2 \\ &\geq 1 - Ce^{-\frac{\delta}{h}}. \end{aligned}$$

The result now follows from the variational principle and (1.1-2). □

It would be interesting to have a more detailed understanding of the optimal exponent δ in Proposition 1.2. In the case of a Schrödinger operator the optimal exponent is given by the Agmon distance between the two wells. A less ambitious problem would be to determine a lower bound for the splitting to complement the upper bound given here. See also [He2] for estimates on the splitting.

Section III.2: The localized operator and the WKB-construction.

The aim of this section is to analyze the first eigenvalue λ_1^i of the localized transfer operator K_i. First we choose the B_i's of the previous section so small that the WKB-construction (at each critical point $1 \leq i \leq k$) of Section I.6 is defined in B_i.

Let $f_N^i \in L^2(B_i)$ be given by

$$f_N^i(x;h) = e^{-\frac{1}{h}\varphi_N^i(x;h)}, \qquad \varphi_N(x;h) = \sum_{k=0}^{N} \varphi_k^i(x) h^k.$$

Here φ^i_k are the WKB-phases associated with the critical point z_i. By the variational principle

$$\begin{aligned}\lambda^i_1 \|f^i_N\|^2_{L^2(B_i)} &\geq \langle f^i_N, K_i f^i_N\rangle_{L^2(B_i)}\\ &\geq e^{-F^i_N(h)-C_N h^{N+1}} \|f^i_N\|^2_{L^2(B_i)},\end{aligned}$$

where

$$F^i_N(h) = \sum_{k=0}^{N} F^i_k h^k$$

and the F^i_k's are the expansion coefficients obtained during the construction of the φ^i_k's.

We will now employ a trick due to Helffer and Ramond [HeRa] to get the opposite inequality. The following estimate holds for all strictly positive ψ

$$\|K_i\|_{\mathcal{B}(L^2(B_i))} \leq \sup_{x\in B_i} \int_{B_i} K(x,y)\frac{\psi(y)}{\psi(x)}dy.$$

This estimate follows from the proof of the Schur Lemma. Choosing $\psi = f^i_N$ gives

$$\lambda^i_1 \leq e^{-F^i_N(h)+C_N h^{N+1}}$$

In other words

Proposition III.2.1. *For each $N \in \mathbb{N}$ there exists $h_0 > 0$ such that*

$$\ln \lambda^i_1 = -F^i_N(h) + O(h^{N+1})$$

for $0 < h \leq h_0$.

Let $\mathcal{F}^{-1} = \{1, \ldots, k\}$ and define for $N \geq 0$ sets

$$\mathcal{F}^N = \{i \in \mathcal{F}^{N-1} : F^N_j \leq F^N_i, \text{ for all } j \in \mathcal{F}^{N-1}\}$$

and

$$\mathcal{F}^\infty = \cap_{N=0}^\infty \mathcal{F}^N \neq \emptyset.$$

Notice that $F^i_N(h) = F^j_N(h)$ for $i, j \in \mathcal{F}^N$ (for $N = \infty$ in the sense of formal power series) and there exists $h_0 > 0$ such that $F^i_N(h) > F^j_N(h)$ for $i \in \mathcal{F}^N$, $j \notin \mathcal{F}^N$ and $0 < h \leq h_0$. Combining this with Theorem 1.1 and Proposition 2.1 we find the following two results.

Theorem III.2.2. *For each $N \in \mathbb{N}$ there exists $h_0 > 0$ such that*

$$\ln \lambda_1 = -F_N^i(h) + O(h^{N+1})$$

for $i \in \mathcal{F}^N$ and $0 < h \leq h_0$.

Corollary III.2.3. *There exists $h_0 > 0$ such that for $0 < h \leq h_0$*

$$\|(1-\chi_\infty)\psi_1\| \leq Ce^{-\frac{\delta}{h}},$$

where $\chi_\infty = \sum_{i \in \mathcal{F}^\infty} \chi_i$.

Proof. Let $\mu_2' = \max_{i \notin \mathcal{F}^\infty} \lambda_1^i$ and estimate, using (1.1-2) and argument similar to the one that gave (1.3),

$$\begin{aligned} \lambda_1 &= \langle \psi_1, K\psi_1 \rangle \\ &\leq \mu_1 \|\chi_\infty \psi_1\|^2 + \mu_2' \|(1-\chi_\infty)\psi_1\|^2 + Ce^{-\frac{\delta}{h}} \\ &= \mu_1 + (\mu_2' - \mu_1)\|(1-\chi_\infty)\psi_1\|^2 + Ce^{-\frac{\delta}{h}}. \end{aligned}$$

By Proposition 2.1 we find that $\mu_1 - \mu_2' \geq Ch^N$, for some $C > 0$ and $N \in \mathbb{N}$, and this together with Theorem 1.1 proves the result. □

In the proof of the next result we will need another version of the μ_2 used in the proof of the previous result. Namely

$$\mu_2'' = \max_{i \in \mathcal{F}^\infty} \{\lambda_2^i\},$$

where the λ_2^i's are the second eigenvalues of the restricted operators K_i (see Theorem 2.5). One can use harmonic approximation to verify that $\lambda_1^i - \lambda_2^i \geq C > 0$ uniformly in small h, see [He5]. Hence we have

$$\mu_1 - \mu_2'' \geq C > 0. \tag{2.1}$$

Proposition III.2.4. *Let $h_0 > 0$ be small enough. For all $0 < h \leq h_0$ there exists $\underline{\omega} = \underline{\omega}(h) = \{\omega_i\}_{i \in \mathcal{F}^\infty}$ with $\omega_i > 0$ and $\sum_{i \in \mathcal{F}^\infty} \omega_i^2 = 1$ such that*

$$\|\psi_1 - \psi_{1,\underline{\omega}}\| \leq Ce^{-\frac{\delta}{h}}, \quad \textit{where} \quad \psi_{1,\underline{\omega}} = \sum_{i \in \mathcal{F}^\infty} \omega_i \psi_1^i.$$

Proof. Let, for $i \in \mathcal{F}^\infty$,

$$\tilde{\omega}_i = \langle \psi_1, \psi_1^i \rangle \quad \text{and} \quad \omega_i = \frac{\tilde{\omega}_i}{\sqrt{\sum_{i \in \mathcal{F}^\infty} \tilde{\omega}_i^2}}.$$

We introduce the subspace $\mathcal{H}_0 \subset L^2(\mathbb{R}^m)$ of linear combinations of the functions ψ_1^i, $i \in \mathcal{F}^\infty$ (extended to 0 outside B_i). Notice that $\varphi \in \mathcal{H}_0^\perp$ will satisfy that $\varphi_{|B_i} \perp \psi_1^i$, for $i \in \mathcal{F}^\infty$. We wish to prove that

$$|\langle \varphi, \psi_1 \rangle| \leq Ce^{-\frac{\delta}{h}} \tag{2.2}$$

for $\varphi \in \mathcal{H}_0^\perp$. This will imply the result since $\psi_{1,\underline{\omega}}$ is exactly the orthogonal projection of ψ_1 onto $\mathcal{H}_0$.

The estimate (2.2) holds by Corollary 2.3 for φ with support outside

$$B_\infty = \cup_{i \in \mathcal{F}^\infty} B_i.$$

As for functions with support inside B_∞ we introduce the projection onto $\mathcal{H}_0$

$$P\varphi = \sum_{i \in \mathcal{F}^\infty} \langle \psi_1^i, \varphi \rangle \psi_1^i$$

and the operator (on $L^2(B_\infty)$)

$$K_\infty = \sum_{i \in \mathcal{F}^\infty} K_i.$$

Notice that $PK_\infty = K_\infty P$ and $I - P$ is the projection onto functions in $\mathcal{H}_0^\perp$ restricted to B_∞. We can now estimate using $K_{\infty | \operatorname{Range}(I-P)} \leq \mu_2''$

$$\begin{aligned} \|(I-P)\chi_\infty \psi_1\|^2 &= \langle (I-P)(\mu_1 - K_\infty)^{-1}(I-P)\chi_\infty\psi_1, (\mu_1 - K_\infty)\chi_\infty\psi_1 \rangle \\ &\leq (\mu_1 - \mu_2'')^{-1} \|(I-P)\chi_\infty\psi_1\| \|(\mu_1 - K_\infty)\chi_\infty\psi_1\|. \end{aligned} \tag{2.3}$$

By (1.2) we have

$$\|K_\infty - \chi_\infty K \chi_\infty\| \leq Ce^{-\frac{\delta}{h}},$$

which we combine with (2.1) and (2.3) to get the estimate

$$\begin{aligned} \|(I-P)\chi_\infty\psi_1\| &\leq C\|(\mu_1 - K_\infty)\chi_\infty\psi_1\| \\ &\leq C\|(\mu_1 - K)\chi_\infty\psi_1\| + Ce^{-\frac{\delta}{h}} \\ &\leq C\|(\mu_1 - K)\psi_1\| + Ce^{-\frac{\delta}{h}}, \end{aligned}$$

where we used Corollary 2.3 in the last step. The result now follows from an application of Theorem 1.1. □

If at least two of the weights ω_i vanishes at most polynomially in h then the splitting between the two first eigenvalues of the transfer operator is $O(h^\infty)$. We omit the proof which follows from Proposition 2.4. See also Proposition 1.2.

Theorem III.2.5. *Suppose $|\mathcal{F}^\infty| = 1$. There exists $h_0 > 0$ such that for $0 < h \leq h_0$*

$$\lambda_2 = \mu_2(1 + O(1)e^{-\frac{\delta}{h}}),$$

where $\mu_2 = \max\{\mu_2', \mu_2''\}$.

Proof. Write $\mathcal{F}^\infty = \{i_0\}$. The first step of the proof is an analogue of the estimate (1.3)

$$\begin{aligned}
\lambda_2 &= \langle \psi_2, K\psi_2 \rangle \\
&\leq \langle \chi_{i_0}\psi_2, K\chi_{i_0}\psi_2 \rangle + \sum_{i \neq i_0} \langle \chi_i\psi_2, K\chi_i\psi_2 \rangle + Ce^{-\frac{\delta}{h}} \\
&\leq \mu_2'' \|\chi_{i_0}\psi_2\|^2 + \mu_2' \|(1-\chi_{i_0})\psi_2\|^2 + Ce^{-\frac{\delta}{h}} \\
&\leq \mu_2 + Ce^{-\frac{\delta}{h}}. \qquad (2.4)
\end{aligned}$$

As for the other inequality we use the variational principle. Let

$$\tilde{\psi}_2^{i_0} = \psi_2^{i_0} - \langle \psi_1, \psi_2^{i_0} \rangle \psi_1$$

and for the other critical points, $i \neq i_0$, we choose

$$\tilde{\psi}_2^{i} = \psi_1^{i} - \langle \psi_1, \psi_1^{i} \rangle \psi_1.$$

Then $\tilde{\psi}_2^i \perp \psi_1$, $1 \leq i \leq k$, and by Proposition 2.4

$$\begin{aligned}
1 \geq \|\tilde{\psi}_2^{i_0}\|^2 &= 1 - |\langle \psi_2^{i_0}, \psi_1 \rangle|^2 \\
&= 1 - |\langle \psi_2^{i_0}, \psi_1 - \psi_1^{i_0} \rangle|^2 \\
&\geq 1 - Ce^{-\frac{\delta}{h}}.
\end{aligned}$$

For $i \neq i_0$ we estimate using Corollary 2.3

$$\begin{aligned}
1 \geq \|\tilde{\psi}_2^{i}\|^2 &= 1 - |\langle \psi_1, \psi_1^{i} \rangle|^2 \\
&\geq 1 - Ce^{-\frac{\delta}{h}}.
\end{aligned}$$

We thus get

$$\lambda_2 \geq \mu_2 - Ce^{-\frac{\delta}{h}},$$

which together with (2.4) and the a priori estimate $\mu_2 \geq C > 0$ uniformly in small $h > 0$ implies the result. One can use harmonic approximation to show the a priori estimate for $\mu_2^{i_0}$, which is a one well problem (see [He5]), and the estimate $\mu_1^i \geq C$ is covered by (1.5) (see Theorem 1.1). $\square$

Section III.3: Globally convex potentials.

In the case where the potential V is globally convex the constructions given in this paper are global as well. In particular the 0'th order phases (in the low-temperature and strong-coupling limits) are also globally convex and if the Hessian of V is bounded uniformly from below or above then so are the 0'th order phases (see Theorems II.1.1 and II.3.5). In the special case where the Hessian of the potential is bounded uniformly from both above and below then one can estimate all the higher order phases globally as well in the sense that they all grow at most linearly at infinity and have uniformly bounded derivatives (provided all derivatives of the potential of order 3 and higher are uniformly bounded). We will not prove this result here for two reasons. The proof is rather technical and lengthy and we will need and extended version of the proof in a later paper in order to show that the WKB-constructions considered here are stable with respect to the standard function class introduced by Sjöstrand (see [Sj2]). Notice that this result underscores that the choice of ansatz for the first eigenfunction employed here is a natural one. We note that one can use such a result to give an alternative proof of Theorem 2.2.

In the case of the strong coupling limit it seems to be necessary to know something about the decay of the first eigenfunction outside wells in order to make a localization argument work. Alternatively one can make the assumption of uniform bounds (from above and below) on the Hessian of V and prove the analogue of Theorem 2.2 in the strong coupling limit using the uniform control of higher order phases.

It is natural to ask wether or not the 0'th order phases can be extended smoothly beyond a region of convexity into a region of attraction where

$$x \cdot V' > 0, \quad \text{for} \quad x \neq 0.$$

In one dimension the eikonal equation (the 0'th order phase in the strong-coupling limit) has the smooth solution

$$\varphi(x) = \operatorname{sign}(x) \int_0^x \sqrt{V(y)}dy.$$

However a numerical test for the one-dimensional potential

$$V(x) = x^2 + \frac{3}{4} x \sin(x)$$

shows that the incoming manifold for the corresponding diffeomorphism κ ceases to be a graph (over configuration space) outside an interval which grows with J (to include more and more regions of non-convexity). The 0'th order low-temperature phase is therefore not a globally smooth function in this example.

Section III.4: Chains of continuous spins.

In this section we will briefly review the consequences of the results of Part III in the context of a ferromagnetic, $J > 0$, system of continuous spins arranged on the one-dimensional lattice $\mathbb{Z}$.

Let $V \in C^\infty(\mathbb{R}^n)$ be a self-energy. It should satisfy the conditions introduced in Section 1 and we suppose for simplicity that it grows at least linearly at infinity. The energy of a spin-distribution at finite volume

$$\Lambda = \{-L, \ldots, L\} \subset \mathbb{Z}, \quad L \in \mathbb{N},$$

is given by

$$H_\Lambda(\underline{\sigma}) = \sum_{i \in \Lambda} V(\sigma_i) + \frac{J}{2} \sum_{i \sim j} |\sigma_i - \sigma_j|^2,$$

where $i \sim j$ means nearest neighbour with the periodic boundary condition $-L \sim L$. The spin distribution $\underline{\sigma}$ takes values in the one-particle space $\mathbb{R}^n$. We note that the quantities discussed here are independent of the choice of boundary condition.

The partition function and free energy of the system is

$$Z_\Lambda(\beta) = \int_{\mathbb{R}^{n|\Lambda|}} e^{-\beta H_\Lambda(\underline{\sigma})} d^{n|\Lambda|}\underline{\sigma}$$

and

$$F_\Lambda(\beta) = -\frac{\ln Z_\Lambda(\beta)}{\beta}.$$

It is well known that in the thermodynamic limit $(L \to \infty)$ we have

$$-\beta \lim_{L \to \infty} F_\Lambda(\beta) = \frac{n}{2} \ln \pi - \frac{n}{2} \ln \beta + \lambda_1(\beta),$$

where λ_1 is the highest eigenvalue of the transfer operator with potential V and coupling constant J. In other words Theorem 2.2 gives a low-temperature expansion of the free energy in the thermodynamic limit.

Other quantities of interest are expectations of the Gibbs measure, which at finite volume is given by

$$d\mu_{\beta,\Lambda} = Z_\Lambda(\beta)^{-1} e^{-H_\Lambda} d^{n|\Lambda|}\underline{\sigma}.$$

Of particular interest is the two-point correlation function

$$\mathrm{cor}_{\beta,\Lambda}(i,j) = \int_{\mathbb{R}^{n|\Lambda|}} \sigma_i \cdot \sigma_j \quad d\mu_{\beta,\Lambda}. \tag{4.1}$$

Another well known connection between the transfer operator and the thermodynamic limit of one-dimensional spin-systems is the following relation

$$\lim_{L\to\infty} \ln \operatorname{cor}_{\beta,\Lambda}(i,j) \sim -\ln\left(\frac{\lambda_1}{\lambda_2}\right)|i-j|,$$

asymptotically for large $|i-j|$. In other words the inverse correlation length of the system is given by the logarithm of the splitting between the two first eigenvalues of the transfer operator. In the case where the self-energy is a symmetric double well we see from Proposition 1.2 that the correlation length can become exponentially large in the low-temperature limit. In the case where $|\mathcal{F}^\infty| = 1$ (in particular in the case of a unique global minimum) one can apply Theorem 2.5 to localize the problem and compute the asymptotics of the correlation lenght at low temperatures using for example harmonic approximation or WKB-analysis. In [BJS] the low-temperature limit of the correlation function (4.1) is determined completely, for $n = 1$, under assumptions on the potential which implies a unique critical point. Here we get the correlation lenght at low-temperatures under much weaker conditions on V.

We refer the reader to [F], [K], [He4] and [He5] for a more thorough discussion of the connection between transfer operators and spin-systems.

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