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Semiclassical Expansions of the Thermodynamic Limit for a Schrödinger Equation

II. The double well case

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Abstract:

We give a proof of the semi-classical expansion of the thermodynamic limit which works also for the double well case. This permits also the study of the splitting between the two first eigenvalues and a partial proof of a conjecture of M.Kac and C.J.Thompson [Ka-Th].

§0 Introduction

This article is motivated by a course of M.Kac [Ka] (see also [Br-He]) and completes the study started in [He-Sj].

Let us first recall the origin of the problem in statistical mechanics. M.Kac proposes to study the following model (called Model A in §7 in [Ka]) whose hamiltonian is given by :

$E_{V(N,M)}(\sigma) = -\Sigma_{(P,Q)\in V\times V}\, v_{P,Q}\, \sigma_P\sigma_Q$

with :

$V(N,M) = [1,\dots,N]\times(\mathbb{Z}/M\mathbb{Z})$ in $\mathbb{Z}^2$, $\sigma_P\in\{-1,+1\}$, $J\in \mathbb{R}_+^*$, $\gamma\in\mathbb{R}_+^*$

$v_{P,P} = 0$

and

$v_{P,Q} = J\gamma \exp(-\gamma|k-k'|)\{\delta_{\ell',\ell} + (1/2)\ (\delta_{\ell',\ell+1}+\delta_{\ell',\ell-1}\}$ if $P=(k,\ell)\neq Q=(k',\ell')$.

M.Kac observes that the free energy per spin in the thermodynamic limit :$-\Psi/kT$ can be computed (see formula (7.11)) as :

$-\Psi/kT = \ln 2 - \nu\gamma/2 + \mathrm{Lim}_{m\leftarrow\infty}(\ln \Lambda_{max}(m)/m)$

where $\Lambda_{max}(m)$ is the largest eigenvalue of the m-dimensional integral operator K given by :

$K = \exp(-Q^{(m)}/2)\exp(-\gamma(-\Delta^{(m)}))\exp(-Q^{(m)}/2)$

with

$Q^{(m)}(y) = (\tanh(\gamma/2)/2)\,\Sigma_{k=1}^{m} y_k^2 - \Sigma_{k=1}^{m}\ln\cosh(\sqrt{\nu\gamma/2}\ (y_k+y_{k+1}))$

and $\nu = J/kT$.

As γ tends to zero, the operator is well approximated by

$\exp(-\gamma(-\Delta^{(m)}) - Q^{(m)})$

(see [Br-He] for rigorous results in this direction or [He]) and it is consequently natural (see (7.17) in [Kac]), after a scaling argument $x_k=\gamma^{1/2}y_k$, to study the problem of the existence and the properties of the limit of $\lambda_1(m;h,\nu)/m$ where $\lambda_1(m;h,\nu)$ is the smallest eigenvalue of

(0.1) $P^{(m)}(x,hD_x;\nu) = -h^2\Delta^{(m)} + V^{(m)}(x;\nu)$

with

(0.2) $V^{(m)}(x;\nu) = (1/4)\,\Sigma_{k=1}^{m} x_k^2 - \Sigma_{k=1}^{m}\ln\cosh(\sqrt{\nu/2}\ (x_k+x_{k+1}))$,

with the convention $(x_{m+1}=x_1)$.

h is essentially equivalent to γ as γ tends to 0 and we finally arrive (after some approximation) to the usual semiclassical problem for a Schrödinger operator. Moreover, the splitting between the second eigenvalue $\lambda_2(m;h,\nu)$ and the first one appears to be strongly connected (see for example formula (7.32) in [Ka]) to the behavior as r tends to ∞ of the behavior of the correlation function of two spins in a row separated by a distance r.

Of course all these connections are not mathematically rigorous but this gives us the motivation for our study of the Schrödinger case.

As already mentioned this study was started in [He-Sj]. More precisely by completing results of $[Sj]_{1,2}$ we treated completely the case where the parameter ν (which in the corresponding statistical problem is the inverse of the temperature) is less than 1/4, assumption which implies the convexity of the potential.

Let us recall the three results which were obtained in this case .

Theorem 0.1 (Cf [He-Sj], $[Sj]_3$)

For every ν *in* $\mathbb{R}^+$ *the limit* $\Lambda(h,\nu) = \mathrm{Lim}_{m\to\infty}\,(\lambda_1(m;h,\nu)/m)$ *exists*

Theorem 0.2 (Cf [He-Sj])

If $\nu < 1/4$, $\Lambda(h,\nu) = \mathrm{Lim}_{m\to\infty}\,(\lambda_1(m;h,\nu)/m)$ *admits a complete asymptotic expansion :*

$\Lambda(h,\nu) \sim h\Sigma_{j\geq 0}\,\Lambda_j(\nu).h^j$ *as h tends to 0.*

Moreover, if we denote the corresponding semiclassical expansions for $\lambda_1(m;h,\nu)/m$ *by :*

$(\lambda_1(m;h,\nu)/m) \sim h\Sigma_{j\geq 0}\,\Lambda_j(m,\nu).h^j$,

there exists $k_0(\nu) > 0$ *s.t. for each j, there exists a constant* $C_j(\nu)$, *s.t.*

$|\Lambda_j(\nu) - \Lambda_j(m,\nu)| \leq C_j(\nu).\exp(-k_0\, m)$.

$k_0(\nu)$ and $C_j(\nu)$ *can be chosen locally independent of* ν .

Theorem 0.3 (cf $[Sj]_2$, [He-Sj])

If $\nu < 1/4$ *then the splitting between the two first eigenvalues* λ_2 *and* λ_1 *is controlled by*

$(h/C_\nu) \leq |\lambda_2(m,h,\nu) - \lambda_1(m,h,\nu)| \leq C_\nu .h$

for some $C_\nu > 0$ *which can be chosen locally independent of* ν .

The purpose of this paper is to complete the description of the properties of the thermodynamic limit and of the splitting in the case where $\nu > 1/4$.
More precisely we shall prove the following theorems :

Theorem 0.4

If $\nu > 1/4$, $\Lambda(h,\nu) = \mathrm{Lim}_{m\to\infty} (\lambda_1 (m;h,\nu) / m)$ *admits a complete asymptotic expansion :*
$\Lambda(h,\nu) \sim \Lambda^0(\nu) + h\Sigma_{j\geq 0} \Lambda_j(\nu).h^j$ *as h tends to 0.*
Moreover, if we denote the corresponding semiclassical expansions for $\lambda_1 (m;h,\nu) / m$ *by :*
$(\lambda_1 (m;h,\nu) / m) \sim \Lambda^0(\nu) + h\Sigma_{j\geq 0} \Lambda_j(m,\nu).h^j$,
there exists $k_0(\nu) > 0$ *s.t. for each j, there exists a constant* $C_j(\nu)$, *s.t.*
$|\Lambda_j(\nu) - \Lambda_j(m,\nu)| \leq C_j(\nu). \exp(-k_0\, m)$.
$k_0(\nu)$ and $C_j(\nu)$ *can be chosen locally independent of* ν .

Remark 0.5

With the corresponding statement of Theorem 0.2 we have the complete answer outside the critical value.

Theorem 0.6

If $\nu > 1/4$ *and let us consider the set in* $\mathbb{N} \times \mathbb{R}^+$ *defined by*
(0.3) $m \leq Ch^{-N_0}$,
(we write shortly $m = O(h^{-N_0})$
for some C and N_0 *;*
then there exists C_ν , h_ν *and* $\varepsilon_\nu > 0$ *such that for all the (m,h) in this set satisfying* $0 < h \leq h_\nu$, *the splitting between the two first eigenvalues* λ_2 *and* λ_1 *is controlled by*
$\lambda_2(m,h,\nu) - \lambda_1 (m,h,\nu) \leq C_\nu . \exp - (\varepsilon_\nu . m / h)$.

Remark 0.7

Here we observe a very different behavior in comparison with the case $\nu < 1/4$ (Theorem 0.3) but we have unfortunately a restriction on m . This is probably a technical difficulty. We were hoping to prove simply that (first conjecture) :

$\mathrm{Lim}_{m\to\infty} (\lambda_2(m,h,\nu) - \lambda_1(m,h,\nu)) = 0.$

This property will be a sign of a " transition of phase" in the following sense. If we assume (second conjecture!) that $\mathrm{Lim}_{m\to\infty}(\lambda_2(m,h,\nu) - \lambda_1(m,h,\nu))$ always exists and that (third conjecture) it is analytic for $\nu < 1/4$, then we get from Theorem 0.3 that this limit is not analytic around 1/4.

In the proof of Theorems 0.4 and Theorem 0.6 we shall follow the same strategy as in $[Sj]_{1,2}$,[He-Sj].

Let us recall that the basic idea in order to analyze the thermodynamic limit was to compare a formal expansion of the eigenvalue (divided by the dimension) (deduced from the WKB approximation whose construction with control with respect to the dimension m was initiated in $[Sj]_{1,2}$) of a one well problem and the first eigenvalue (divided by the dimension) of our problem . We can distinguish three parts.

In the first one, one compares the WKB approximation of the one well problem and the first eigenvalue of the Dirichlet problem in a sufficiently small ℓ^∞ - ball around the point where the minimum of the potential was attained.

In the second one we compare the first eigenvalue of the Dirichlet problem in this small ℓ^∞ - ball with the global problem.

In these two steps we work modulo $m.O_N(h^N)$ (for any N) but the dimension is controled by $m = O(h^{-N_0})$.

The last part is to eliminate the restriction on the dimension and is identical to the convex case (due to the control of the convergence in the thermodynamic limit).

In fact we shall prove a more precise result permitting to analyze the splitting between the two first eigenvalues. To understand what is needed recall the following classical formula for the splitting (see for example [He-Sj], §3) :

$$(0.4)\ \lambda_2 - \lambda_1 = \mathrm{Inf}_\phi\{ [(\int |h\nabla\phi|^2 (u_{1,m})^2(x)\,dx)/\int|\phi|^2 (u_{1,m})^2(x)\,dx)],\quad \phi\in C_0^\infty, \int\phi\,(u_{1,m})^2(x)\,dx = 0\}$$

Here $u_{1,m}$ denotes the first normalized eigenfunction.

The estimates about the splitting are then deduced from the choice of ϕ and of information on the decay of $u_{1,m}$ in suitable domains. We observe that under the assumption $\nu > 1/4$, the potential admits two minima and that there exists δ s.t. the region $\Omega(\delta)$ defined by :

(0.5) $\Omega(\delta) = \{x \in \mathbb{R}^m, -\delta \leqslant \Sigma_i x_i \leqslant \delta\}$

does not contain these two wells. Let us recall also that according to the symmetries of the problem we have :

(0.6) $u_{1,m}(-x) = u_{1,m}(x)$

Let $\chi(t)$ be a C^∞ function s.t.

$(0.7)_1$ $\chi(t) = -\chi(-t)$

$(0.7)_2$ $0 \leqslant \chi(t) \leqslant 1$ for $t \geqslant 0$.

$(0.7)_3$ $\chi(t) = 1$ for $t \geqslant 1$.

Taking

(0.8) $\phi_\delta(x) = \chi(\Sigma x_i/\delta)$

(ϕ is not with compact support but the argument can be easily completed by density), we deduce from (0.4) the following estimate :

(0.9) $\lambda_2(m,h) - \lambda_1(m,h) \leqslant C_\nu . m . h^2 . (\alpha(m,h)^2/(1-\alpha(m,h)^2)$

with

(0.10) $\alpha(m,h,\delta) = \|u_{1,m}\|_{L^2(\Omega(\delta))}$

Theorem 0.6 will be a consequence of the following theorem which will be proved in section 3 :

Theorem 0.8

There exists $\tilde{C}$, h_0 and $\delta > 0$ s.t.

(0.11) $\alpha(m,h,\delta) \leqslant \tilde{C} \exp(-m/\tilde{C}h)$

if (0.3) is satisfied and $0 < h < h_0$.

§1. WKB approximation in a ℓ^∞-ball

As mentioned in the introduction, one first step corresponds to the study of the problem in a small neighborhood of some minimum of the potential.

The remark is the following : what we have made in [He-Sj] (adapting previous results of $[Sj]_{1,2}$) works also for $\nu > 1/4$.

For this we return to the verification in §6.2 of [He-Sj] of the conditions given in §4 of the same article to obtain the Theorem 4.4 and the assumptions in $[Sj]_{1,2}$ to compare with Dirichlet problems in some ball.

If $\nu > 1/4$, let us observe that we have two wells. Let us start by recalling briefly what we shall get from the study of the harmonic approximation at the bottom (see §2).

We shall see that we have two equal minimas at $\pm x^c(m,\nu)$ with $x^c(m,\nu) = (t^c/2)(1,\ldots\ldots,1)$ and let us now work in a small ℓ^∞-neighborhood of say $x^c(m,\nu)$.

Let us verify carefully the different assumptions following section 6 in [He-Sj].

We shall verify the following properties for the potential $V = V^{(m)}$.

(1.1) There exist d and k (independent of m) s.t. V is holomorphic in $B_\infty(x^c,d)$ with $|\nabla V(x)|_\infty = O(1)$,

(1.2) $V''(x^c) = D + A$, where D is diagonal (positive definite) and $\|A\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} \leq r_1 < r_0 \leq \lambda_{min}(D)$ for all p s.t. $1 \leq p \leq \infty$ and for all ρ with :

(*) $\exp(-\mathscr{k}) \leq \rho(j+1)/\rho(j) \leq \exp(\mathscr{k})$.

(1.3) $\|\nabla^2 V\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} = O(1)$ uniformly in $B_\infty(x^{\mathscr{k}},d)$ for ρ satisfying (*).

(1.4) $V^{(m)\,''}(x) \geq ((1-4\nu'')/2\,).\, I_m$ for x in $B^{\mathbb{R}}_\infty(x^c,d)$ with $\nu' < \nu'' < 1/4$.

Here $(1-4\nu')/2$ is the smallest eigenvalue of $V^{(m)\,''}(x^c)$ (which appears to be independent of m, see (2.8)).

With $\mathscr{W}^m_n = V^{(m)} - (V^{(n)} \tilde{\oplus} V^{(m-n)})$ $(1 \leq n \leq m-1)$, we must have :

(1.5) For all m, for all n $((1 \leq n \leq m-1))$, for all ρ defined on $\{1,\ldots\ldots,m\}$ and satisfying (*) and

(**) $\rho(j) = 1$ for $j \geq n+1$, and $\rho(1) = 1$,

we have uniformly with respect to ρ, m, n :

$|\nabla \mathscr{W}^m_n|_{\ell^\infty_\rho} = O(1)$ in a complex ball $B(x^c,d)$.

(1.6) $V^{(m)}$ and more generally $(1-t)\,(V^{(n)} \tilde{\oplus} V^{(m-n)}) + t\, V^{(m)}$ for $0 \leq t \leq 1$ satisfy (1.1)-(1.2) uniformly for the ρ satisfying (*) and (**) (more generally (*) and

(***)
$$\exp(-\mathscr{k}) \leq \rho(n)/\rho(1) \leq \exp(\mathscr{k})$$
$$\exp(-\mathscr{k}) \leq \rho(m)/\rho(n+1) \leq \exp(\mathscr{k})\,)$$

Here
$(V^{(n)} \tilde{\oplus} V^{(m-n)})(x_1, \ldots, x_m) = V^{(n)}(x_1, \ldots, x_n) + V^{(m-n)}(x_{n+1}, \ldots, x_m)$.

(1.7) For every m, $V^{(m)}$ satisfies :
$V^{(m)}(x_m, x_1, \ldots, x_{m-1}) = V^{(m)}(x_1, \ldots, x_m)$.

The verification of (1.1) is easy. We first observe (always with the convention that $x_{m+1} = x_1$) that :
(1.8) $\partial_{x_i} V^{(m)}(x) =$
$= (x_j/2) - \sqrt{\nu/2}\ \mathrm{th}\ (\sqrt{\nu/2}\ (x_j + x_{j+1})) - \sqrt{\nu/2}\ \mathrm{th}\ (\sqrt{\nu/2}\ (x_j + x_{j-1}))$
and that if $|x - x^c|_\infty$ is $\leqslant r$,
$|\sqrt{\nu/2}\ (x_j + x_{j+1} - t^c)| \leqslant r\sqrt{2\nu}$
According to the analyticity of $t \to \mathrm{th}\ t$ in the neighborhood $B(t^c, d_0)$ of t^c we just choose d s.t.
(1.9) $d\sqrt{2\nu} < d_0/2$
and under this condition $\partial_{x_i} V^{(m)}(x)$ is bounded independently of m.

Let us observe for future use that :
(1.10) $(\partial^2_{x_i} V^{(m)})(x) =$
$= ((1/2) - \nu) + (\nu/2)[\mathrm{th}^2(\sqrt{\nu/2}\ (x_j + x_{j+1})) + \mathrm{th}^2\ (\sqrt{\nu/2}\ (x_j + x_{j-1}))$
(1.11) $\partial_{x_j} \partial_{x_{j+1}} V^{(m)}(x) =$
$= -\nu/2\ (1 - \mathrm{th}^2\ (\sqrt{\nu/2}\ (x_j + x_{j+1}))) = -\nu/(2 \cosh^2\ (\sqrt{\nu/2}\ (x_j + x_{j+1})))$
(1.12) $\partial_{x_j} \partial_{x_k} V^{(m)}(x) = 0$ if $|j-k| \neq 0, -1, +1$ modulo m.

For (1.2) we deduce from §2. :
(1.13) $D = ((1/2) - \nu')\ I_m$
where I_m is the identity in $\mathbb{R}^m$, so we have :
(1.14) $r_0 = \lambda_{min}(D) = ((1/2) - \nu')$.
If we denote by τ the operator on $\mathbb{R}^m$ defined by: $(\tau x)_i = x_{i-1}$, we can write :
(1.15) $A = -(\nu'/2)\ (\tau + \tau^{-1})$
The eigenvalues of A are easily computed as $-\nu' . \cos(2\pi k/m)$ for $k = 0, 1, \ldots, m-1$.
It is then easy to verify that for ρ satisfying to (*) :
(1.16) $\|A\|_{\mathcal{L}(\ell^p_\rho, \ell^p_\rho)} \leqslant \nu' . \exp(k)$

Because $\nu' < 1/4$, we observe that one can choose $\mathscr{k}$ such that:

(1.17) $r_1 = \nu'.\exp(\mathscr{k}) < ((1/2) - \nu')$

and we shall make this choice now.

The proof of (1.3) is immediate if we observe that all the second derivatives are bounded and that we have (1.12).

(1.4) is a consequence of (1.11)–(1.12) by choosing d small enough:

(1.18) $0 < d \leqslant d_1(\nu',\nu'')$

Let us now verify (1.5). We just observe that:

$$\mathscr{W}_n^m = \ln\cosh(\sqrt{\nu/2}\ (x_m + x_1)) + \ln\cosh(\sqrt{\nu/2}\ (x_n + x_{n+1}))$$
$$- \ln\cosh(\sqrt{\nu/2}\ (x_n + x_1)) - \ln\cosh(\sqrt{\nu/2}\ (x_m + x_{n+1}))$$

The only j for which $\partial_{x_j}\mathscr{W}_n^m$ are not 0 are $j = 1, n, n+1, m$

and using 1.11 one has for each of these terms:

$|\partial_{x_j}\mathscr{W}_n^m(x)| \leqslant 4\sqrt{\nu/2}\ \mathrm{Sup}_{\tau \in B(t^c, d_0)}\ (\mathrm{th}(\sqrt{2\nu}\ \tau)$

for $x \in \mathbb{C}^m$, $|x - x^c|_\infty \leqslant d$.

According to the (**), the property (1.5) is clear.

Let us verify (1.6). We first observe that:

$D_t^{(m)} = (1-t)\, D^{(n)} \oplus D^{(m-n)} + t\, D^{(m)}$

and:

$A_t^{(m)} = (1-t)\, A^{(n)} \oplus A^{(m-n)} + t\, A^{(m)}$.

All the properties we need are stable by arithmetical means, so it is sufficient to treat the case $(V^{(n)} \tilde{\oplus} V^{(m-n)})$ for ρ satisfying (***) and (*) which can be reduced by separation of variables to the study of $V = V^{(m)}$ for ρ satisfying (*).

We now observe that $\lambda_{min}(D) = (1/2) - \nu'$ and that $\|A\| \leqslant \nu'.\exp(\kappa)$.

Because $\nu' < 1/4$, it is easy to choose $\kappa > 0$ s.t:

$\nu'.\exp(\kappa) < (1/2) - \nu')$.

Finally (1.7) is clear from the definition.

Conclusion

If we take d satisfying the two conditions (1.10) and (1.18), we have a complete analysis of the first eigenvalue of the Dirichlet problem modulo $O(h^{\infty})$ but under the condition (0.3).

We shall need the same properties for $V^{(m)}$ replaced by

$\tilde{V}^{(m),N} = V^{(m)} - \Sigma_j (x_j - (t^c/2))^{2N}$.

By symmetry we have also the same properties near $-x^c(m,\nu)$.

§2.The harmonic approximation in the case $\nu > 1/4$.

Following Kac, we observe that :

(2.1) $$V^{(m)}(x) = (1/16)\Sigma_{k=1}^{m}(x_k - x_{k+1})^2 + $$
$$+ (1/16)\Sigma_{k=1}^{m}(x_k + x_{k+1})^2 - \Sigma_{k=1}^{m} \ln\cosh(\sqrt{\nu/2}\ (x_k + x_{k+1})).$$

(with the convention $x_{m+1} = x_1$).

and we can write :

(2.2) $$V^{(m)}(x) = (1/16)\Sigma_{k=1}^{m}(x_k - x_{k+1})^2 + $$
$$+ \Sigma_{k=1}^{m} q((x_k + x_{k+1}),\nu)$$

with

(2.3) $q(t,\nu) = (1/16)\ t^2 - \ln\cosh(\sqrt{\nu/2}\, t)$

To find the minimas we observe that :

(2.4) $V^{(m)}(x) \geq m.\min q$

If $\nu > 1/4$,

(2.5) q admits two equal minimas at $\pm t^c$ $(t^c > 0)$

where t^c satisfies

(2.6) $t^c = 4\sqrt{2\nu}\ \ \mathrm{th}(\sqrt{\nu/2}\, t^c)$.

It is then easy to see that there are only two points in $\mathbb{R}^m$ s.t. we have equality in (2.4) and we get the

Lemma 2.1

If $\nu > 1/4$, the minimum of $V^{(m)}$ is equal to m.min q and is only attained at the following two points:

(2.5) $$x^c_{\pm}(m,\nu) = \pm x^c(m,\nu) \quad \text{with } x^c = (t^c/2)\ (1,1,1,\dots.,1).$$

Approximation at the bottom.

At x^c, this approximation is given by :

(2.6) $Q_0(\overline{x}) = (1/4)\,\Sigma_{k=1}^{m}\,\overline{x}_k^{\,2} - (\nu'/4)\,(\Sigma_{k=1}^{m}(\overline{x}_k+\overline{x}_{k+1})^2\,)$

where we have written :

(2.7) $x = \overline{x} + x^c$

and

(2.8) $\nu' = \nu\big(1-\mathrm{th}^2(\sqrt{\nu/2}\;\;t^c)\big)$

Here we observe that $\nu' < 1/4$, and that the quadratic approximation is the same as for $\nu < 1/4$ but with ν replaced by ν'.

This is well analyzed in [Ka]. We shall prove later (see also manuscript [He]) that the harmonic approximation is valid and in particular that the first eigenvalue of the Schrödinger equation is approximated modulo $O(mh^2)$ by $m.\mathrm{Min}q + h(1/2\pi)\int_0^{\pi}\sqrt{-4\nu'.\cos^2\theta}\;d\theta$.

§3. Exponentially weighted estimates for the eigenfunctions.

As a preparation we consider $f(t) = \ln\big(\mathrm{ch}\;(\sqrt{(\nu/2)}\;t)\big)$ so that $f(t)$ is an even strictly convex function with the asymptotic behavior

(3.1) $f(t) \approx \sqrt{(\nu/2)}\;t - \ln 2 + O(\exp(-t/C),\; t \to +\infty.$

If $x,y \in \mathbb{R}$, we have $f(x-y)-f(x+y) = f(|x-y|) - f(|x+y|)$,

and we first assume that :

$|y| \leqslant |x|$ and $xy \leqslant 0$.

Then $|x+y| \leqslant |x-y|$ and $|x-y|-|x+y| = 2|y|$.

Hence

$$f(|x-y|) - f(|x+y|) \sim |y|\;.\;|x-y|\;/\;(1+|x-y|)$$
$$\sim |y|.\max\,(|x|,|y|)/(1+\max\,(|x|,|y|))\;.$$

Here we have the convention that $a \sim b$ with a and b >0 (depending of different parameters) , if (a/b) and (b/a) are bounded uniformly.

In the general case, we then get :

(3.2) $f(|x+y|)-f(|x-y|) \sim \mathrm{sgn}\,(xy)\;.\;\min(|x|,|y|).\max\,(|x|,|y|)/(1+\max\,(|x|,|y|))$

and if we assume that $\max(|x|,|y|) \geqslant$ Const. >0, we obtain :

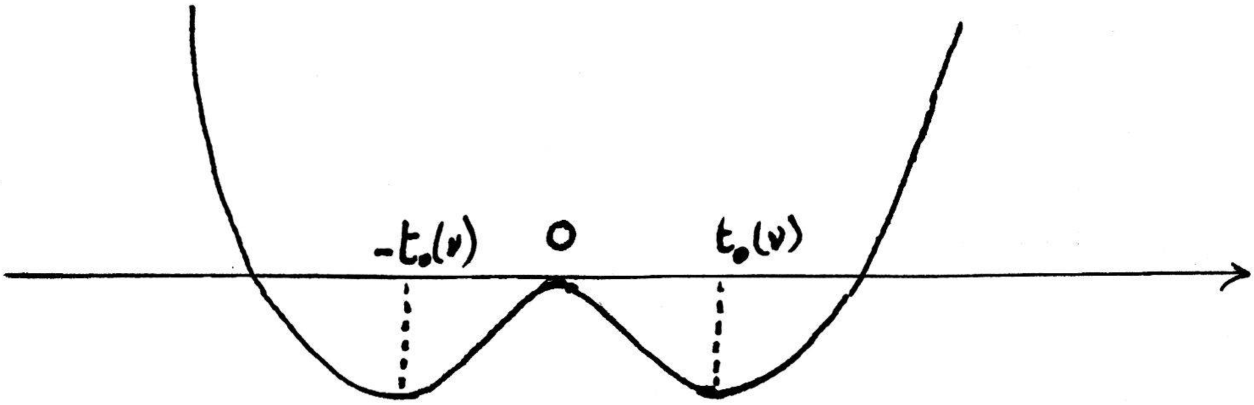
(3.3) $f(|x+y|) - f(|x-y|) \sim \mathrm{sgn}\,(xy)\;.\;\min(|x|,|y|)$.

We shall use the fact (see §2) that

(3.4) $V(x) = (1/16)\Sigma_{k=1}^{m}(x_k - x_{k+1})^2 +$
$$+\Sigma_{k=1}^{m} v((x_k + x_{k+1})/2) = (1/4)(\Sigma_k x_k^2) - \Sigma_{k=1}^{m} f((x_k + x_{k+1})/2)$$
with

(3.5) $v(t) = q(2t,\nu) = (1/4)\,t^2 - \ln\cosh(\sqrt{2\nu}\ t)$

and recall that for $\nu > 1/4$, v has a double well with two minimas at $\pm\, t_0(\nu)$ with $t_0(\nu) > 0$.



Let $0 < \varepsilon_0 << \delta_0 << 1$ and consider two types of intervals in $\mathbb{R}$:

Type 1.

$I = I_+ = [t_0 - \delta_0, t_0 + \delta_0]$ or

$I = I_- = [-t_0 - \delta_0, -t_0 + \delta_0]$.

These intervals correspond to neighborhoods of the wells of v.

Type 2

$I = [t - \varepsilon_0, t + \varepsilon_0]$ with $|t - t_0| \geqslant \delta_0 - \varepsilon_0$ and $|t + t_0| \geqslant \delta_0 - \varepsilon_0$.

If I is of the second type then $\pm t_0 \notin I$.

Let us remark also that one can cover $\mathbb{R}$ with intervals of this type.

We want to estimate the lowest eigenvalue of the Dirichlet realization of $-h^2\Delta + V$ in $\Omega = \Pi_1^m I_j$ where I_j is of type 1 or 2 for every j. We write :
$I_j >_{\varepsilon_0} 0$ if $I_j \subset]\varepsilon_0, \infty[$, $I_j \geqslant_{\varepsilon_0} 0$ if $I_j \subset]-2\varepsilon_0, \infty[$. We say that (j,k) with $j,k \in \mathbb{Z}/m\mathbb{Z}$ is a change of sign for a given Ω if $I_j >_{\varepsilon_0} 0$, $I_k <_{\varepsilon_0} 0$ or $I_j <_{\varepsilon_0} 0$, $I_k >_{\varepsilon_0} 0$ and if $I_\nu \ni_{\varepsilon_0} 0$ (that is I_ν meets $[-\varepsilon_0, \varepsilon_0]$) for all $\nu \in]j,k[=_{\mathrm{def}} \{j+1, j+2, \ldots, k-1\}$.

(We define similarly [j,k[,]j,k], [j,k] and write for instance $j<\nu\leqslant k$ if $\nu\in]j,k]$).
Let us observe that the number of changes of sign is even.
Let (j_1,k_1) and (j_2,k_2) be two consecutive changes of sign so that $j_1<k_1\leqslant j_2<k_2\leqslant j_1$. Then consider the map κ from $\mathbb{R}^m$ into $\mathbb{R}^m$:
$x \to \tilde{x} = \kappa(x)$
with
$\tilde{x}_\nu = -x_\nu$ for $k_1 \leqslant \nu \leqslant j_2$, $\tilde{x}_\nu = x_\nu$ for all other ν.
For $x\in\Omega$, we consider

$$
\begin{aligned}
V(x)-V(\kappa(x)) &= [-f((x_{k_1-1}+x_{k_1})/2)+f((x_{k_1-1}-x_{k_1})/2)] \\
&\quad +[-f((x_{j_2}+x_{j_2+1})/2)+f((x_{j_2}-x_{j_2+1})/2)] \\
&= \mathcal{J}_1+\mathcal{J}_2.
\end{aligned}
$$

If $j_1=k_1-1$, then either $I_{k_1-1}<_{\varepsilon_0}0$, $I_{k_1}>_{\varepsilon_0}0$ or $I_{k_1-1}>_{\varepsilon_0}0$, $I_{k_1}<_{\varepsilon_0}0$, and the $\mathcal{J}_1$ can be bounded (using 3.3) from below by $(1/C(\varepsilon_0))=\beta_0\,\varepsilon_0^{\,2}$ where $\beta_0>0$.
If $j_1\neq k_1-1$, then $I_{k_1-1}\ni_\varepsilon 0$ and $\mathcal{J}_1\geqslant -\beta_1\varepsilon_0$ for some constant β_1 (we observe here that f is globally Lipschitzian).
The same discussion holds for $\mathcal{J}_2$ where we distinguish between the cases $k_2=j_2+1$ and $k_2\neq j_2+1$.
Let us call the change of sign (j,k) <u>strict</u> if $k=j+1$.

Applying the same procedure several times, we get a map
$\kappa\colon \Omega=\Pi_1^m I_j \to \Pi_1^m \tilde{I}_j=\tilde{\Omega}$
$x\to\kappa(x)=\tilde{x}$ with $\tilde{x}_j=\pm x_j$, $\tilde{I}_j=\pm I_j$
such that $\tilde{I}_j\geqslant_{\varepsilon_0}0$ and such that for $x\in\Omega$:
(3.6) $V(x)-V(\kappa(x)) \geqslant (\alpha_+(\Omega)/C(\varepsilon_0)) - \alpha_0(\Omega)\,\beta_1\varepsilon_0$.
Here $\alpha_+(\Omega)$ is the number of strict changes of sign and $\alpha_0(\Omega)$ is the number of I_j's meeting $[-\varepsilon_0,\varepsilon_0]$. Notice that $\alpha_0(\tilde{\Omega})=\alpha_0(\Omega)$.
Now consider $\Omega=\Pi_1^m I_j$ with $I_j\geqslant_{\varepsilon_0}0$. Let x_j^Ω be the midpoint of I_j and set $x^\Omega=(x_1^\Omega,\ldots\ldots,x_m^\Omega)$.
Let $\kappa\colon \Omega\to\Omega_+=(I_+)^m$ be the translation with $\kappa(x^\Omega)=x^{\Omega_+}$.
Using (3.4), we see that for $x\in\Omega$:
(3.7) $V(x)-V(\kappa(x)) \geqslant (\beta(\Omega)/C(\delta_0))$
where $\beta(\Omega)$ is the number of I_j which do not contain t_0 (or $-t_0$). Notice that $\beta(\Omega)$ is unchanged by the first "κ".
We now compose our two maps, notice that $\alpha_0(\Omega)\leqslant\beta(\Omega)$ and choose ε_0 so

small that $\varepsilon_0 << C(\delta_0)^{-1}$. We then get a new map $\kappa(x)$ being the composition of reflexions in 0 in some of the coordinates and a translation such that

$\kappa: \Omega \to \Omega_+$, ($\Omega$ is the original box)

$\kappa(x^{\Omega}) = x^{\Omega_+}$ and

(3.8) $V(x) - V(\kappa(x)) \geq (1/C)\ (\alpha_+(\Omega)+\beta(\Omega)),\ x \in \Omega.$

C is here a strictly positive constant, independent of Ω, once we have fixed ε_0 and δ_0 conveniently as explained before.

Let P_Ω denote the Dirichlet realization of $-h^2\Delta+V$ in Ω and let μ_+ denote the lowest eigenvalue of P_{Ω_+}. Let μ_0 denote the lowest eigenvalue of $-h^2\Delta+V$ on $\mathbb{R}^n$. By the minimax principle, we have

(3.9) $\mu_0 \leq \mu_+$

and recall from section 1 that, under the assumption $m = O(h^{-N_0})$, we have a good knowledge of the asymptotics for μ_+ deduced from WKB constructions.

(3.8) shows that :

(3.10) $P_\Omega - \mu_+ \geq (1/C)\ (\alpha_+(\Omega) + \beta(\Omega)).$

Since all our maps take the mid point of the boxes into mid points of the image-boxes, we also get (cf $[Sj]_{1,2}$, [He-Sj]), **under the assumption** $\mathbf{m = O(h^{-N_0})}$:

(3.11) $P_\Omega - \Sigma_1^m (x_j - x_j^\Omega)^{2M} - \mu_+^M(h) \geq (1/C)\ (\alpha_+(\Omega) + \beta(\Omega))$ if $\Omega \neq \Omega_\pm$.

with a new constant $C>0$, where

(3.12) $\mu_+^M(h) - \mu_+(h) = O(h^{N(M)})$

with $N(M)$ tending to ∞ with $M \in \mathbb{N}$ and $h>0$ sufficiently small.

From this point we can imitate the argument of $[Sj]_{1,2}$ and we only recall the main steps . We have a C^∞ positive function ψ_Ω with

(3.13) $|\nabla\psi_\Omega(x)|^2 \leq (1/2)\ \Sigma_1^m (x_j - x_j^\Omega)^{2M},\ \psi_\Omega(x^\Omega) = 0,$

χ_Ω in $C_0^\infty(\Omega)$ and a measure $\mu(d\Omega)$ such that

(3.14) $\int \chi_\Omega(x)^2 .\ \exp(-2\psi_\Omega(x)/h)\ \mu(d\Omega) = 1 + O(\exp(-1/Ch))$

where O is uniform with respect to x.

We first show that :

(3.15) $\mu_+^M \leq \mu_0 + O(h^\infty).$

Let $\mu < \mu_+^M$; we have

$$(3.16)\ ((P-\mu)\chi_\Omega \exp(-\psi_\Omega/h)u|\chi_\Omega \exp(-\psi_\Omega/h)u) = (\chi_\Omega \exp(-\psi_\Omega/h)(P-\mu)u|\chi_\Omega \exp(-\psi_\Omega/h)u) + ((h\nabla(\chi_\Omega \exp(-\psi_\Omega/h))^2 u|u)$$

which can be written as

$$(3.17)\ ((P-\mu-|\nabla\psi_\Omega|^2)\chi_\Omega \exp(-\psi_\Omega/h)u|\chi_\Omega \exp(-\psi_\Omega/h)u) = (\chi_\Omega \exp(-\psi_\Omega/h)(P-\mu)u|\chi_\Omega \exp(-\psi_\Omega/h)u) + ((h^2|\nabla\chi_\Omega|^2 - 2h\chi_\Omega\nabla\chi_\Omega.\nabla\psi_\Omega)\exp(-\psi_\Omega/h)u|\exp(-\psi_\Omega/h)u).$$

Combining with (3.12) and (3.13), we get :

$$(\mu_+^M - \mu)\|\chi_\Omega \exp(-\psi_\Omega/h)u\|^2 \leqslant (\chi_\Omega \exp(-\psi_\Omega/h)(P-\mu)u|\chi_\Omega \exp(-\psi_\Omega/h)u) + ((h^2|\nabla\chi_\Omega|^2 - 2h\chi_\Omega\nabla\chi_\Omega.\nabla\psi_\Omega)\exp(-\psi_\Omega/h)u|\exp(-\psi_\Omega/h)u).$$

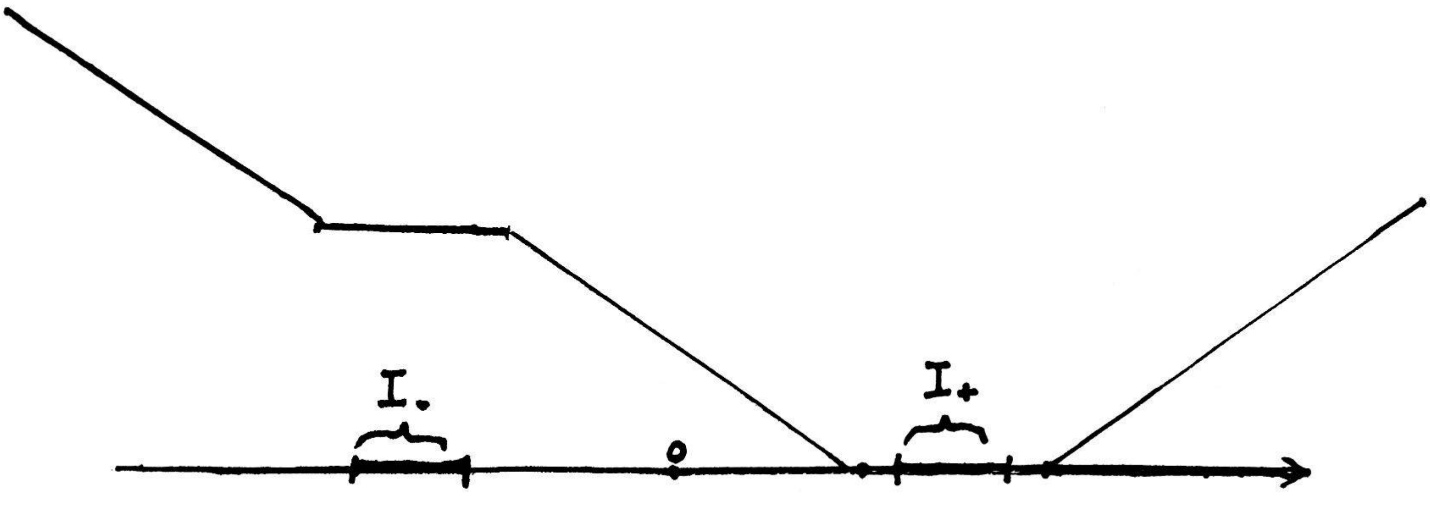
Integrating with respect to $\mu(d\Omega)$ gives :

$$(\mu_+^M - \mu)(1+O(\exp(-1/Ch))\|u\|^2 \leqslant \leqslant \big(1+O(\exp(-1/Ch))\big).(P-\mu)u|u) + O(\exp(-1/Ch)\ \|u\|^2.$$

We then take $\mu = \mu_0$ and get (3.15) and finally (playing with arbitrary M and using (3.9) and (3.12)) :

(3.18) $\mu_0 = \mu_+ + O(h^\infty)$ (under the condition $m = O(h^{-N_0})$).

We next look at exponentially weighted estimates. Let $\Psi_+(t)$ be a positive function with the shape :



So that $\Psi_+ = 0$ near I_+ ,

$\Psi_+ = \alpha > 0$ near I_-

and Ψ_+ has a small constant slope (in absolute value) outside.

Put $\Psi_-(t) = \Psi_+(-t)$,

(3.19) $\phi(x) = \text{Inf}\ (\Sigma_1^m \Psi_+(x_j), \Sigma_1^m \Psi_-(x_j))$.

Then $\phi|_{\Omega_+} = 0$ and

(3.20) $|\vec{\nabla}\phi(x)|^2 \leqslant (1/3C)(\beta(\Omega))$ if $x \in \Omega$.

Let u be the positive normalized eigenfunction associated to μ_0 :

$(P-\mu)\, u = 0$. Put $\phi_\Omega(x) = \phi(x) - \Psi_\Omega(x)$.

Then

$$((P-\mu_0)\chi_\Omega \exp(\phi_\Omega/h)u|\chi_\Omega \exp(\phi_\Omega/h)u) = (|h\nabla(\chi_\Omega \exp(\phi_\Omega/h)|^2 u|u)$$

which we write as

(3.21) $$((P-\mu_0 - |\nabla\phi_\Omega|^2)\chi_\Omega \exp(\phi_\Omega/h)u|\chi_\Omega \exp(\phi_\Omega/h)u) = ((2h\chi_\Omega\nabla\chi_\Omega.\nabla\phi_\Omega + h^2|\nabla\chi_\Omega|^2)\exp(\phi_\Omega/h)u|\chi_\Omega \exp(\phi_\Omega/h)u)$$

Here $|\nabla\phi_\Omega|^2 \leqslant 2|\nabla\phi|^2 + 2\,|\nabla\Psi_\Omega|^2$ and combining (3.13), (3.20), (3.14), (3.21) and (3.16), we get when $\Omega \neq \Omega_\pm$:

(3.22) $$\|\chi_\Omega \exp(\phi_\Omega/h)u\|^2 \leqslant C\,((2h\chi_\Omega\nabla\chi_\Omega.\nabla\phi_\Omega + h^2|\nabla\chi_\Omega|^2)\exp(\phi_\Omega/h)u|\chi_\Omega \exp(\phi_\Omega/h)u)$$

and integrating with respect to $\mu(d\Omega)$, we get :

(3.23) $$\int(1 + O(\exp(-1/Ch))\exp(2\phi/h)|u|^2 dx \leqslant O(\exp(-1/Ch))\|\exp(\phi/h)u\|^2 + \|u\|^2_{\Omega_+} + \|u\|^2_{\Omega_-}$$

which implies :

(3.24) $\|\exp(\phi/h)u\|^2 = O(1)$ (under the condition $m = O(h^{-N_0})$).

Let $x \in \mathbb{R}^m$. Let " $2I_+$ " and "$2I_-$" denote the intervals with the same mid points as I_+ and I_- but with double lengths. We notice that for some $\tilde{\alpha} > 0$:

$\Psi_+(t) \geqslant \tilde{\alpha}\,\mathrm{dist}(t, 2I_+) \geqslant \tilde{\alpha}\,(|t - t_0| - 2\delta_0)$.

Hence $$\Sigma_1^m x_j = \Sigma_1^m (x_j - t_0) + m\,t_0 \geqslant -\Sigma_1^m |x_j - t_0| + m\,t_0 \geqslant -\Sigma_1^m (|x_j - t_0| - 2\delta_0) + m\,t_0 - 2m\delta_0 \geqslant -\Sigma_1^m \Psi_+(x_j)/\tilde{\alpha} + (t_0 - 2\delta_0).m\,.$$

So

$\Sigma_1^m \Psi_+(x_j) \geqslant \tilde{\alpha}\,(t_0 - 2\delta_0).m - \tilde{\alpha}\,|\Sigma_1^m x_j|$.

The same estimate holds for $\Sigma_1^m \Psi_-(x_j)$ so

$\mathrm{Min}\,(\Sigma_1^m \Psi_+(x_j), \Sigma_1^m \Psi_-(x_j)) \geqslant \alpha\,(t_0 - 2\delta_0).m - \tilde{\alpha}\,|\Sigma_1^m x_j|$.

We have $t_0 - 2\delta_0 > 0$ and for m large enough we have finally

(3.25) $\mathrm{Min}\,(\Sigma_1^m \Psi_+(x_j), \Sigma_1^m \Psi_-(x_j)) \geqslant (1/C)\,m$

f

(3.26) $\Sigma_1^m x_j \in [-1,+1]$.

Then, according to (3.19), and (3.24), Theorem 0.8 is a immediate consequence of (3.25).

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