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Semiclassical expansions of the thermodynamic limit for a Schrödinger equation

I. The one well case

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§1 Presentation of the problem :

One of the motivations of the study presented here is a statistical model introduced by M.Kac [Ka]₂ and called the exponential bidimensional model. This model was supposed to present phase transition. Let us just recall here (see [Ka]₂ or [Br-He] for details) that after some reductions M.Kac arrive to the question of studying the spectral properties of the following operator:

$$(1.1) K_m(h) = \exp[-V^{(m)}(x)/2] \cdot \exp[h^2 \sum_{k=1}^m \partial^2 / \partial x_k^2] \cdot \exp[-V^{(m)}(x)/2]$$

with¹ :

$$(1.2) V^{(m)}(x) = (1/4) \sum_{k=1}^m x_k^2 - \sum_{k=1}^m \log \operatorname{ch}(\sqrt{v/2} (x_k + x_{k+1})).$$

¹ In fact, the operator which appears in Kac is $\exp(-mh/2)K_m(h)$. It is easier w.l.o.g. in this article to work with this modified Kac operator.

The parameter ν is here the inverse of the temperature and h is a semi-classical parameter. The two questions of interest are in this context:

(1.3) If $\mu_1(m;h,\nu)$ is the largest eigenvalue of the Kac's operator, what is the behavior as a function of ν and h of the thermodynamic quantity :

$$\lim_{m \rightarrow \infty} (-\text{Log } \mu_1(m;h,\nu) / m).$$

(1.4) If $\mu_2(m;h,\nu)$ is the second eigenvalue (which is $< \mu_1(m;h,\nu)$ by standard results), can we study the quantity :

$$\lim_{m \rightarrow \infty} (\mu_2(m;h,\nu) / \mu_1(m;h,\nu)).$$

From discussions with specialists in statistical mechanics (with T.Spencer for example), we get the impression that this problem is probably well understood and that according to the value of ν with respect to a critical value ν_c the answer to (1.4) will be that the limit will be < 1 for $\nu < \nu_c$ and will be 1 for $\nu > \nu_c$. This is a sign of a transition of phase. However, we do not have a precise reference for that and at least the problem of analyzing in detail the behavior of the different thermodynamic quantities near the critical value ν_c seems to remain open.

In his interesting course in Brandeis [Ka]₂, M. Kac explains, at least heuristically, how to compare (in the semi-classical context) the operator $K_m(h)$ to the exponential of (minus) a Schrödinger operator. The validity of this approximation (for m fixed) has been studied more carefully in [He-Br] and [He] using some results of [He-Sj]_{1,4}.

If we admit this approximation, we shall find the following problems for the Schrödinger equation :

$$(1.5) P_m(h) = -\sum_{k=1}^m h^2 \partial^2 / \partial x_k^2 + V^{(m)}(x).$$

(1.6) If $\lambda_1^{(m)}(h, \nu)$ is the smallest eigenvalue of the Schrödinger's operator, study as a function of ν and h the thermodynamic quantity :

$$\text{Lim}_{m \rightarrow \infty} (\lambda_1(m; h, \nu) / m).$$

(1.7) If $\lambda_2(m; h, \nu)$ is the second eigenvalue (which is $> \lambda_1(m; h, \nu)$ by standard results), study the quantity :

$$\text{Lim}_{m \rightarrow \infty} (\lambda_2(m; h, \nu) - \lambda_1(m; h, \nu)).$$

Forgetting the initial Kac's problem, we shall start to study in this article these two questions (1.6) and (1.7). Because it is a high dimension problem, we shall use (at least in the semi-classical context) the techniques introduced by one of us (J.S). Most of the results which are given here :

- (1) existence of the thermodynamic limit $\text{Lim}_{m \rightarrow \infty} (\lambda_1(m; h, \nu) / m)$
- (2) asymptotic expansion of the limit as a formal series in h
- (3) rapidity of the convergence as $m \rightarrow \infty$

are given in a relatively general framework but we shall see how it can be applied in our motivating example, in the particular case where $\nu < \nu_c$.

This is of course just the starting point (and the easiest) of a study which has to consider after the case where $\nu > \nu_c$, and then the transition around $\nu = \nu_c$. There is some hope to return later to the initial Kac's problem. This ν_c can be guessed by looking carefully to the properties of $V^{(m)}$. As observed by V.Kac, for $\nu < 1/4$, the potential $V^{(m)}$ has a unique minimum at 0 and appears to be convex. For $\nu > 1/4$, we shall observe a double well problem which is certainly more difficult to analyze.

The principal result of this paper will be :

Theorem 1.1

If $\nu < 1/4$, the limit $\Lambda(h, \nu) = \lim_{m \rightarrow \infty} (\lambda_1(m; h, \nu) / m)$ exists and admit a complete asymptotic expansion :

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

Moreover, if we denote the corresponding semiclassical expansions for

$\lambda_1(m; h, \nu) / m$ by :

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

there exists κ_0 s.t. for each j , there exists a constant $C_j(\nu)$, s.t.

$$|\Lambda_j(\nu) - \Lambda_j(m, \nu)| \leq C_j(\nu) \cdot \exp(-\kappa_0 m).$$

$C_j(\nu)$ can be chosen independently of ν in a compact of $[0, 1/4[$.

The problems, we consider here, are also connected to quantum field theory problems and a lot of results have been obtained by other techniques (see for example the new edition of [Gl-Ja] for a updated presentation).

The paper is organized in three parts.

The first part (§ 2 and §3) is essentially devoted to the proof of the existence of the thermodynamic limit. This is a non-semiclassical proof but we shall see that a control of the convergence with respect to parameters can be useful. In §3 we give additional remarks (to [Sj]₂) on universal estimates of the splitting of the two first eigenvalues .

The second part (§4 and §5) is the semi-classical part and the natural continuation of two papers by one of us (J.S) [Sj]_{1,2}.

In the last part (§6), we shall first recall some preliminary computations by Kac [Ka] and then deduce the Theorem 1.1 as a particular case of the more general results obtained in the preceding sections.

The first author (B.H) thanks V.Tchoulaevski and T.Spencer for useful remarks and stimulating discussions.

§2 On the existence of the thermodynamic limit $\lambda_1(m)/m$

This section is inspired by the reading of the book of Ruelle [Ru] which gives probably the necessary ideas to extend the results we present here to more general interactions.

Let us just consider the following model :

$$(2.1) P_m = -\hbar^2 \Delta_m + \sum_{k=1}^m W(x_k, x_{k+1})$$

(with the convention that $m+1=1$)

operating on $L^2(\mathbb{R}^m)$.

Here :

$$(2.2) \Delta_m = \sum_{k=1}^m (\partial_{x_k})^2$$

We forget the semi-classical problem (we take $\hbar=1$) (but if needed the proof will be sufficiently explicit to have a control with respect to \hbar), we assume that W is C^∞ and satisfies :

$$(2.3) W \geq 0$$

There exists a constant $C_0 > 0$ s.t.:

$$(2.4) \quad W(t,s) \leq C_0 (W(t,r) + W(u,s)+1) \text{ for all } t,s,r,u \in \mathbb{R}$$

which will be called the decoupling inequality.

Moreover, we assume

$$(2.5) \quad W(t,s) \rightarrow \infty \text{ as } |t|+|s| \rightarrow \infty.$$

This last property (which is not necessary at all) permits us to work in the simpler context where the Schrödinger equation has compact resolvent.

Remark 2.1 :

(2.4) and (2.5) follow from the stronger assumptions, that there exists constants $C_1, C_2 > 0$, and C_3 s.t. :

$$(2.6) \quad W(t,s) \geq (1/C_2) (t^2 + s^2) - C_1 \text{ for all } s,t \in \mathbb{R}$$

$$(2.7) \quad W(t,s) \leq C_2 (t^2 + s^2) + C_3 \text{ for all } s,t \in \mathbb{R}$$

We shall denote in this section by $\lambda(m) = \lambda_1(m)$ the first eigenvalue of P_m . This first eigenvalue always exists (the resolvent is compact) and we shall denote by u_m the corresponding eigenfunction uniquely determined if we suppose that the L^2 norm is one and that u_m is positive. Recall that by standard results u_m is strictly positive.

The main result of this section is the following :

Theorem 2.2

Under the assumptions (2.3) – (2.5), the sequence $\lambda(m)/m$ is convergent as m tends to infinity.

Majoration. minoration :

We get from (2.3) that :

$$(2.8) \lambda(m) \geq 0$$

and (2.4) (with $r = u = 0$) and (2.5) imply :

$$(2.9) \lambda(m) \leq C m$$

We then have :

$$(2.10) \quad 0 \leq \text{Lim inf}_{m \rightarrow \infty} \lambda(m)/m \leq \text{Lim sup}_{m \rightarrow \infty} \lambda(m)/m < \infty$$

The following simple lemma will play a crucial role

Lemma 2.3

There exists a constant C_4 such that, for all $m \geq 1$, we have, for $j = 1$ to m :

$$(2.11) \quad \|W(x_j, x_{j+1})^{1/2} u_m\|^2 \leq \lambda(m)/m \leq C_4$$

Proof :

From (2.3), we get :

$$\sum_j \|W(x_j, x_{j+1})^{1/2} u_m\|^2 \leq \lambda(m)$$

We observe now that the potential is invariant by circular permutation. By usual arguments, we get that u_m (which is strictly positive and corresponds to an eigenvalue of multiplicity 1) has the same property.

In particular $\|W(x_j, x_{j+1})^{1/2} u_m\|^2$ is independent of j . The lemma follows immediately with $C_4 = \text{Sup}_m (\lambda(m)/m)$.

Comparison between $\lambda(m)$, $\lambda(p)$ and $\lambda(m+p)$

In a second step we shall prove the

Lemma 2.4

There exists a constant $C_5 > 0$ such that, for all integers m, p s.t. $1 \leq p, 1 \leq m$, we have :

$$(2.12) \quad -C_5 + \lambda(m) + \lambda(p) \leq \lambda(m+p) \leq C_5 + \lambda(m) + \lambda(p)$$

Proof

We start from the following decomposition of P_{m+p}

$$(2.13) \quad P_{m+p} = P_m + \hat{P}_p^{(m+1)} - W(x_m x_1) + W(x_m x_{m+1}) - \\ - W(x_{m+p} x_{m+1}) + W(x_{m+p} x_1)$$

$$\text{with : } \hat{P}_p^{(m+1)} = - \hat{\Delta}_p^{(m+1)} + \sum_{k=m+1}^{m+p-1} W(x_k x_{k+1}) + W(x_{m+p} x_{m+1})$$

$$\text{and } \hat{\Delta}_p^{(m+1)} = \sum_{k=m+1}^{m+p} (\partial_{x_k})^2$$

It is then clear that the infimum of the spectrum of $\hat{P}_p^{(m+1)}$ is the same as the infimum of P_p . Sometimes we shall use the notation

$$P_m \tilde{\otimes} P_p \text{ instead as } P_m + \hat{P}_p^{(m+1)}.$$

For the minoration of $\lambda(m+p)$, one writes :

$$\lambda(m+p) = (P_{m+p} u_{m+p} | u_{m+p}) \geq (P_m u_{m+p} | u_{m+p}) + (\hat{P}_p^{(m+1)} u_{m+p} | u_{m+p}) \\ - \|W^{1/2}(x_m x_1) u_{m+p}\|^2 - \|W^{1/2}(x_{m+p} x_{m+1}) u_{m+p}\|^2$$

and we use (2.4) and Lemma 2.3.

By the definition of $\lambda(m)$ (and identifying P_m on $L^2(\mathbb{R}^m)$ and $P_m \otimes I$ on $L^2(\mathbb{R}^m) \otimes L^2(\mathbb{R}^p)$ who have the same spectrum (as a set)) we get the first estimate :

$$\lambda(m+p) \geq \lambda(m) + \lambda(p) - C_5 \quad (\text{with } C_5 = 2C_4).$$

For the majoration of $\lambda(m+p)$, we proceed similarly using the fonction:

$$\hat{u}_{p,m}(x) = u_m(x_1, \dots, x_m) u_p(x_{m+1}, \dots, x_{m+p})$$

We have :

$$\lambda(m+p) \leq (P_{m+p} \hat{u}_{m,p} | \hat{u}_{m,p}) \leq (P_m \hat{u}_{m,p} | \hat{u}_{m,p}) + (\hat{P}_p^{(m+1)} \hat{u}_{m,p} | \hat{u}_{m,p}) \\ + \|W^{1/2}(x_m x_{m+1}) \hat{u}_{m,p}\|^2 + \|W^{1/2}(x_{m+p} x_1) \hat{u}_{m,p}\|^2$$

$$\leq \lambda(m) + \lambda(p) + C_5$$

(using the same type of arguments)

The last lemma to prove the proposition is the following :

Lemma 2.5 :

Let C some fixed constant ($C \geq 0$). Let $\lambda(m)$ ($m \in \mathbb{N}^*$) be a sequence of real numbers such that

$$(2.14) \quad |\lambda(m+p) - \lambda(m) - \lambda(p)| \leq C, \text{ for each } m, p,$$

then the limit of the sequence $\lambda(m)/m$ exists and :

$$(2.15) \quad |(\lambda(m)/m) - \text{Lim}_{m \rightarrow \infty} (\lambda(m)/m)| \leq C/m.$$

Proof

Let $\mu(m) = \lambda(m)/m$. Let us rewrite (2.14) on the form :

$$(2.16) \quad |\mu(m+p) - ((m/(m+p))\mu(m)) - ((p/(m+p))\mu(p))| \leq C/(m+p)$$

In particular, for $p = m$, we get :

$$|\mu(2m) - \mu(m)| \leq C/2m$$

and by iteration :

$$|\mu(2^{k+1}m) - \mu(2^k m)| \leq C/(2^k m).$$

In particular $\bar{\mu}(m) := \text{Lim}_{k \rightarrow \infty} \mu(2^k m)$ exists and

$$(2.17) \quad |\bar{\mu}(m) - \mu(m)| \leq C/m.$$

Replacing m and p in (2.16) by $2^k m$ and $2^k p$ and taking the limit in k , we get :

$$(2.18) \quad \bar{\mu}(m+p) = ((m/(m+p))\bar{\mu}(m)) + ((p/(m+p))\bar{\mu}(p)).$$

We now define $\bar{\lambda}(m)$ by : $\bar{\lambda}(m) = m \bar{\mu}(m)$, and rewrite (2.17) as :

$$(2.19) \quad \bar{\lambda}(m+p) = \bar{\lambda}(m) + \bar{\lambda}(p).$$

This implies in particular that $\bar{\lambda}(m) = m\bar{\lambda}(1)$ and then :

$$(2.20) \quad \bar{\mu}(m) = \bar{\mu}(1).$$

(2.17) and (2.20) give the lemma.

Examples

Example 2.6 ([Ka])

Let us consider

$$V_m(x_1, \dots, x_m) = (1/4) \sum_{k=1}^m x_k^2 - \sum_{k=1}^m \log \operatorname{ch}(\sqrt{v} (\sqrt{\xi} x_k + \sqrt{1-\xi} x_{k+1})),$$

where $\xi \in]0,1[$, $v > 0$.

Then this potential can be written on the form (2.1) by taking :

$$W(s,t) = (1/8) (s^2 + t^2) - \log \operatorname{ch}(\sqrt{v} (\sqrt{\xi} t + \sqrt{1-\xi} s))$$

In the introduction we took and in the future we shall take $\xi = 1/2$.

Example 2.7

One gets another example by taking the quadratic approximation at a minimum of the preceding model. Then we arrive to:

$$W(s,t) = (1/16) (s-t)^2 + \mu (s+t)^2$$

where μ depends on v but remains > 0 .

In this case, very explicit computation can be made (see [Ka] or § 6).

Example 2.8

More generally, T.Spencer indicates to one of us (B.H) that the following more general model is interesting :

$$W(s,t) = g(s^2 + t^2) + h (s-t)^2 + \lambda (f(\mu s) + f(\mu t))$$

where $|f(v)| \leq C(|v|+1)$ and $g > 0$ and $h > 0$ are parameters.

Remark 2.9

It is important to remark that for the application to semi-classical analysis there exists at each step of the proofs in this section a very good control with respect to the different constants.

Remark 2.10

It will be interesting in the case of the Examples (2.6) or (2.7) to have a control of the regularity of the limit with respect to the parameter v . It is clear that the convergence is uniform with respect to v , on each compact of $]0, \infty[$, so it is clear that the limit is continuous. Moreover we observe that $(\partial \lambda(m, v) / \partial v) / m$ is a bounded set (by the Hellman's formula) which implies that the limit as m tends to ∞ of $\lambda(m, v) / m$ is Lipschitzian in $]0, \infty[$. But a more interesting result would be to study the properties of analyticity with respect to v . One suspects of course that the limit is analytic with respect to v , for $v < v_c$, in the model presented in the introduction ($\xi = 1/2$, in Example (2.6)).

Remark 2.11 (stability by perturbation)

The limit is relatively stable by perturbation. For example, if we consider the following operator

$$P_m = -\Delta_m + \sum_{k=1}^{m-1} W(x_k, x_{k+1})$$

and if we denote by $\lambda^1(m)$ the first eigenvalue of P_m ,

then it is possible to prove, under the additional assumption that

there exists a constant C s.t., for all $\varepsilon > 0$, we have:

$$(2.21) \quad W(s,t) \leq (1+\varepsilon) (W(s,r) + W(p,t)) + (C/\varepsilon)$$

for all s,t,r,p , that :

$$(2.22) \quad \text{Lim}_{m \rightarrow \infty} \lambda'(m)/m = \text{Lim}_{m \rightarrow \infty} \lambda(m)/m$$

§3 Additional remarks on the splitting of the two first eigenvalues

Let us recall the problem mentioned in (1.7). It is also interesting to have theorems on $\text{Lim}_{m \rightarrow \infty} (\lambda_2(m) - \lambda_1(m))$ and $\overline{\text{Lim}}_{m \rightarrow \infty} (\lambda_2(m) - \lambda_1(m))$. If the potential depends on a parameter ν (typically the inverse of the temperature in Example (2.6)), one is interested in knowing for which values of ν we have :

$$\text{Lim}_{m \rightarrow \infty} (\lambda_2(m;\nu) - \lambda_1(m;\nu)) > 0$$

or

$$\text{Lim}_{m \rightarrow \infty} (\lambda_2(m;\nu) - \lambda_1(m;\nu)) = 0.$$

We shall not give an answer to the most interesting questions in this paper but we shall recall and improve some results obtained in this context. Let us first recall the :

Proposition 3.1 (cf [SWYY])

If V is a C^∞ positive potential tending to ∞ as $|x|$ tends to ∞ , then we have :

$$(3.2) \quad (\lambda_2(m) - \lambda_1(m)) \leq 4 \lambda_1(m)/m$$

We shall now show how to give a result which is more sensible to the property of the Hessian of the potential V . The proposition is the following:

Proposition 3.2

Under the additional assumption that $x \rightarrow (\text{Hess } V)(x)$ is bounded, we have:

$$(3.3) \lambda_2 - \lambda_1 \leq \sqrt{2} \text{ Inf}_{X \in \mathbb{R}^n, \|X\|=1} (\text{Sup}_x (\text{Hess } V)_x(X, X))^{1/2}$$

Proof

The proof is as in [SWWY] reminiscent of the proof of the Payne–Polya–Weinberger inequality [P–P–W]. Similar ideas are used in the paper by B.Simon [Si]₃ who refers to [Ka–Th], §3.

Let u_m^1 the first normalized, strictly positive eigenfunction attached to $\lambda_1(m)$. We forget now the reference to m . Then we have :

$$(3.4) (-\Delta + V) u^1 = \lambda_1 u^1$$

Let :

$$\rho_\ell = \int x_\ell (u^1)^2 dx$$

and let us consider :

$$u^{1,\ell} = (x_\ell - \rho_\ell) u^1$$

$u^{1,\ell}$ is orthogonal to u^1 and by the minimax principle we have :

$$(3.5) \lambda_2 \leq \langle (-\Delta + V) u^{1,\ell} | u^{1,\ell} \rangle / \langle u^{1,\ell} | u^{1,\ell} \rangle \text{ for } \ell \in \{1, \dots, m\}$$

Let us observe now that, as a consequence of :

$$(-\Delta + V) u^{1,\ell} = \lambda_1 u^{1,\ell} - 2\partial_{x_\ell} u^1,$$

we get :

$$\langle (-\Delta + V) u^{1,\ell} | u^{1,\ell} \rangle \leq \lambda_1 \langle u^{1,\ell} | u^{1,\ell} \rangle + 1.$$

Now the uncertainty principle gives :

$$(3.6) \quad (1/2) \leq \|\partial_{x_\ell} u^1\| \|u^{1,\ell}\|,$$

and then finally :

$$(3.7) \quad 0 < \lambda_2 - \lambda_1 \leq 1 / \langle u^{1,\ell} | u^{1,\ell} \rangle$$

and

$$(3.8) \quad \lambda_2 - \lambda_1 \leq 4 \|\partial_{x_\ell} u^1\|^2.$$

Summing over ℓ and using the equation we obtain first Proposition 3.1.

We now observe that (because u^1 is real) for all $\ell \in \{1, \dots, m\}$, we have:

$$(3.9) \quad u_\ell^1 := \partial_{x_\ell} u^1 \text{ is orthogonal to } u^1$$

Similarly to the proof of (3.5), we deduce :

$$(3.10) \quad \lambda_2 \leq \langle (-\Delta + V) u_\ell^1 | u_\ell^1 \rangle / \langle u_\ell^1 | u_\ell^1 \rangle \text{ for } \ell \in \{1, \dots, m\}$$

Let us observe now that :

$$(-\Delta + V) u_\ell^1 = \lambda_1 u_\ell^1 - (\partial_{x_\ell}^2 V) u^1$$

and that :

$$\langle (-\Delta + V) u_\ell^1 | u_\ell^1 \rangle \leq \lambda_1 \langle u_\ell^1 | u_\ell^1 \rangle + (1/2) \langle (\partial_{x_\ell}^2 V) u^1 | u^1 \rangle.$$

Finally we get

$$(3.11) \quad \lambda_2 - \lambda_1 \leq (1/(2 \langle u_\ell^1 | u_\ell^1 \rangle)) \text{Sup}_x \partial_{x_\ell}^2 V$$

Then we take the product of (3.8) and (3.11) to get :

$$(3.12) \quad \lambda_2 - \lambda_1 \leq \sqrt{2} (\text{Sup}_x \partial_{x_\ell}^2 V)^{1/2}.$$

This gives the proposition by observing that all the assumptions are invariant by rotation in \mathbb{R}^m .

Example 3.3 (cf Example 2.6):

If $V_v = \sum_j W_v(x_j, x_{j+1})$, with :

$$W_v(s, t) = (1/8) (s^2 + t^2) - \log \operatorname{ch}(\sqrt{v/2} (t+s))$$

then we get :

$$\lambda_2 - \lambda_1 \leq 1$$

If we introduce the semi-classical parameter h , we shall obtain :

$$\lambda_2 - \lambda_1 \leq h.$$

To finish this section let us give shortly (in the case of \mathbb{R}^m) some universal minoration for the splitting. This result was already proved in [Sj]₂ in the case of an open bounded convex set Ω and it is not difficult to extend the result to the case of \mathbb{R}^m by taking the limit of Dirichlet problems in balls Ω_R of increasing radius R and using the fact that the two first eigenvalues of the Dirichlet problem $\lambda_1^D(\Omega_R)$ (resp. $\lambda_2^D(\Omega_R)$) converge as R tends to ∞ to the corresponding eigenvalues of the global problem in \mathbb{R}^m $\lambda_1(m)$ (resp. $\lambda_2(m)$).

Proposition 3.4 ([Sj]₂):

Let V be a strictly convex C^∞ positive potential tending to ∞ as $|x|$ tends to ∞ . Then we have :

$$(3.13) \quad \lambda_2 - \lambda_1 \geq \sqrt{2} \cdot \inf_x \lambda_{\min}(\operatorname{Hess} V)^{1/2}(x)$$

where $\lambda_{\min}(\operatorname{Hess} V)^{1/2}(x)$ is the smallest eigenvalue of $(\operatorname{Hess} V)^{1/2}(x)$.

To see the interest of such a result let us observe the following :

Lemma 3.5 (Example 2.6)

If $V_\nu = \sum_{j=1}^m W_\nu(x_j, x_{j+1})$, with :

$$W_\nu(s, t) = (1/8) (s^2 + t^2) - \log \operatorname{ch}(\sqrt{(\nu/2)} (t+s)),$$

then the potential is convex iff $\nu \leq 1/4$.

1/4 is consequently the good candidate to be the critical ν_c .

Remark 3.6

The existence of a minoration in the convex case was apparently known to some specialists (as T.Spencer indicated to one of us (B.H.)) at least in the framework of the field theory but surprisingly we do not know a reference before $[Sj]_2$. Recall also that a semiclassical version appears in $[Sj]_1$.

Let us now sketch here a variant (in the case of \mathbb{R}^m) of the proof given in $[Sj]_2$. The first step is the following formula for the splitting (cf for example $[Ki-Si]$)

$$(3.14) \quad \lambda_2 - \lambda_1 = \operatorname{Inf}_\phi \{ [(\int |\nabla \phi|^2 (u^1)^2(x) dx) / \int |\phi|^2 (u^1)^2(x) dx)], \\ \phi \in C_0^\infty, \int \phi (u^1)^2(x) dx = 0 \}$$

This is just a variant of the minimax principle.

The second step is the

Proposition 3.7 (cf [BL]):

Let us assume that $V(x) = (1/2)\omega^2 x^2 + U(x)$ with $\omega \geq 0$ and U convex.

Then

$$g(x) := -\text{Log}(u^1)(x) = (\omega x^2 / \sqrt{2}) + v(x)$$

with v convex .

This step was also basic in the proof in [Sj]₂ (cf also [SWYY] for a proof based on the maximum principle).

For the last step let us introduce some notations. If ϕ is for example a continuous bounded function we can introduce :

$$\langle \phi \rangle = \int \phi (u^1)^2(x) dx, \quad \text{var}(\phi) = \langle (\phi - \langle \phi \rangle)^2 \rangle.$$

Then Brascamp and Lieb give in [Bra-Li] the following inequality :

$$(3.15) \quad \text{var}(\phi) \leq \langle (\nabla \phi | g''_{xx}^{-1} | \nabla \phi) \rangle.$$

The proof is then easy by combining the results of the three steps.

Application 3.8 (Example (2.6))

As seen in Lemma 3.5, Example (2.6) satisfies all the assumptions. In particular we get for all m , and all $v < 1/4$:

$$(3.16) \quad \lambda_2(m;v) - \lambda_1(m;v) \geq \sqrt{(1-4v)}$$

This gives us an interesting control with respect to the temperature. Of course, this result is not astonishing for the specialists in statistical physics.

If the semi-classical parameter h is introduced we get :

$$(3.17) \quad \lambda_2(m;h,v) - \lambda_1(m;h,v) \geq \sqrt{(1-4v)} h.$$

The most interesting result would be to prove that, for $v > 1/4$, the splitting $(\lambda_2(m;h,v) - \lambda_1(m;h,v))$ tends to 0 as m tends to infinity. On the other hand we do not know if, for $v < 1/4$, the limit $(\lambda_2(m;h,v) - \lambda_1(m;h,v))$ exists .

§ 4. Exponentially weighted estimates in the construction of the phase

In this section, we shall develop some complements to the results in [Sj]_{1,2}.

To come back to the notations used in these papers, we shall now work with the operator $-(\hbar^2/2)\Delta_m + V$. Let us introduce a set \mathcal{A} as the disjoint union over \mathbb{N} of sets \mathcal{A}_m :

$$\mathcal{A} = \cup_{m \in \mathbb{N}} \mathcal{A}_m$$

where $\mathcal{A}_m \subseteq \mathcal{V}_m \times \mathcal{R}_m$, \mathcal{V}_m is the set of C^∞ potentials on \mathbb{R}^m and \mathcal{R}_m is the set of applications from $\{1, \dots, m\}$ in \mathbb{R}^+ .

Let us make on \mathcal{A} the following assumptions :

For all (V, ρ) in \mathcal{A}

(4.1) V is holomorphic in $B(0,1)$ with $|\nabla V(x)|_\infty = O(1)$ uniformly in \mathcal{A} and $B(0,1)$, (Here $B(0,1)$ is the open unit ball in \mathbb{C}^m with respect to the norm $|x|_\infty = \sup |x_j|$)

(4.2) $V(0) = 0, V'(0) = 0,$

$V''(0) = D + A$, where D is diagonal (positive definite) and

(4.3) There exists r_1 and r_0 (independent of (V, ρ) in \mathcal{A}) such that :

$$\|A\|_{\mathcal{L}(\ell_p^p, \ell_p^p)} \leq r_1 < r_0 \leq \lambda_{\min}(D)$$

for all p s.t. $1 \leq p \leq \infty$.

We also assume :

$$(4.4) \|\nabla^2 V\|_{\mathcal{L}(\ell_p^p, \ell_p^p)} = O(1)$$

uniformly in \mathcal{A} and p .

Here we write :

$$|x|_{p,\rho} = |\rho x|_p = (\sum \rho(j) |x_j|^p)^{1/p} \text{ for } 1 \leq p < \infty$$

and

$$|x|_{\infty, \rho} = |\rho x|_{\infty} = \text{Sup}_j |\rho(j)x_j|.$$

Because A and $\nabla^2 V$ are symmetric, we deduce from (4.3) and (4.4) that we have the same estimates with ρ replaced by $(1/\rho)$, so we may assume that :

$$(4.5) \quad (V, \rho) \in \mathcal{A} \Rightarrow (V, 1/\rho) \in \mathcal{A}.$$

From this, we get by interpolation that we may assume without loss of generality :

(4.6) If (V, ρ) is in \mathcal{A}_m , $(V, 1)$ is in \mathcal{A}_m where " 1 " is the constant weight defined by $\rho(j) = 1$ for $1 \leq j \leq m$.

As in [Sj]₂ (Lemma 1.1), we see that :

$$(4.7)_1 \quad (V''(0))^{1/2} = \tilde{D} + \tilde{A}$$

with \tilde{D} diagonal and

$$(4.7)_2 \quad \|\tilde{A}\|_{\mathcal{X}(e_p^p, e_p^p)} \leq \tilde{r}_1 < \tilde{r}_0 \leq \lambda_{\min}(\tilde{D})$$

for all p s.t. $1 \leq p \leq \infty$ and uniformly in \mathcal{A} .

The property (4.6) permits to apply the results of [Sj]₂. In particular, let

ϕ_0 be the solution of the eikonal equation :

$$(4.8) \quad (1/2) |\nabla \phi_0|_2^2 = V$$

constructed in [Sj]₂, §2 for $|x|_{\infty} < r$. Then we have the following :

Lemma 4.1

If r is sufficiently small, then we have :

$$(4.9) \quad \|\phi_0''(x)\|_{\mathcal{X}(e_p^p, e_p^p)} = O(1)$$

uniformly for (V, ρ) in \mathcal{A} and for $|x|_{\infty} < r$.

Proof.

We recall first that $\phi_0''(0) = V''(0)^{1/2}$ and that $|\nabla\phi_0''(x)|_\infty = O(1)$. Contrary to the situation in [Sj]_{1,2}, it seems that we will have to work with ϕ_0'' directly (and not just with the Cauchy inequalities to estimate the Hessian from the gradient as in [Sj]₁ §1). Let $q = \xi^2/2 - V$. If we differentiate the H_q flow, we get² :

$$(4.10) \quad \partial_t(\delta x) = \delta \xi, \quad \partial_t(\delta \xi) = V''(x) \cdot \delta x$$

Consider an integral curve $]-\infty, 0] \ni t \rightarrow (x(t), \xi(t))$ of H_q with :

$(x(t), \xi(t)) \rightarrow (0, 0)$ when $t \rightarrow -\infty$, $x(0) = x$, $\xi(0) = \nabla\phi_0(x)$, $|x| < r$ with r small. Recall from [Sj]₂ (§2, 2.16) that³

$$(4.11) \quad |x(t)|_\infty \leq \exp(-|t|/C) |x|_\infty$$

Let $A(t) = \phi_0''(x(t))$. Let Λ_{ϕ_0} be the lagrangian manifold defined by $\{(x, \xi), \xi = \nabla\phi_0(x)\}$. Then the tangent space $T_{(x(t), \xi(t))}(\Lambda_{\phi_0})$ is given by :

$$(4.12) \quad \delta \xi = A(t) \cdot \delta x$$

and if we use that the tangent bundle $T(\Lambda_{\phi_0})$ is invariant under the differentiated H_q -flow we get by taking the t -derivative of (4.12) and using (4.10) :

$\partial_t \delta \xi = \partial_t A(t) \cdot \delta x + A(t) \partial_t \delta x = \partial_t A(t) \cdot \delta x + A(t)^2 \delta x = V''(x) \delta x$, and consequently:

² If we denote by $x(t, y, \eta), \xi(t, y, \eta)$ the solution starting of the point (y, η) at $t = 0$, the equation means :

$$\begin{aligned} \partial^2 x_\rho / \partial t \partial y_j &= \partial \xi_\rho / \partial y_j, & \partial^2 \xi_\rho / \partial t \partial y_j &= \sum_m \partial^2 V / \partial x_\rho \partial x_m \cdot \partial x_m / \partial y_j \\ \partial^2 x_\rho / \partial t \partial \eta_j &= \partial \xi_\rho / \partial \eta_j, & \partial^2 \xi_\rho / \partial t \partial \eta_j &= \sum_m \partial^2 V / \partial x_\rho \partial x_m \cdot \partial x_m / \partial \eta_j \end{aligned}$$

³ we recall that $x(t)$ is an integral curve of $\nabla\phi_0$.

$$(4.13) \partial_t A(t) + A(t)^2 = V''(x(t)).$$

Put $A(t) = V''(0)^{1/2} + B(t)$. Then (4.13) becomes :

$$(4.16) \partial_t B(t) + \mathcal{V}^p(B(t)) = V''(x(t)) - V''(0) - B(t)^2$$

where

$$(4.17) \mathcal{V}^p(B) = V''(0)^{1/2} B + B \cdot V''(0)^{1/2}$$

Here we notice that by the Cauchy inequalities :

$$(4.18) \|V''(x(t)) - V''(x(0))\|_{\mathcal{X}(\ell_p^p, \ell_p^p)} = O(|x(t)|_\infty) = O(1) \exp(-|t|/C).$$

Moreover

$$(4.19) \exp(t \mathcal{V}^p)(B) = \exp(t V''(0)^{1/2}) \cdot B \cdot \exp(t V''(0)^{1/2})$$

and as in [Sj]₂ (Proposition 1.2) we see that :

$$(4.20) \|\exp(t V''(0)^{1/2})\|_{\mathcal{X}(\ell_p^p, \ell_p^p)} \leq \exp(-|t|/C), \text{ for } t \leq 0.$$

Hence :

$$(4.21) \|\exp(t \mathcal{V}^p)(B)\|_{\mathcal{X}(\ell_p^p, \ell_p^p)} \leq \exp(-2|t|/C) \|B\|_{\mathcal{X}(\ell_p^p, \ell_p^p)}, \text{ for } t \leq 0.$$

From (4.16) we get :

$$(4.22) B(t) = \int_{-\infty}^t \exp(-(t-s) \mathcal{V}^p) (V''(x(s)) - V''(0) - B(s)^2) ds$$

If $M(t) = \text{Sup}_{-\infty < s \leq t} \|B(s)\|_{\mathcal{X}(\ell_p^p, \ell_p^p)}$, then

$$(4.23) M(t) \leq C (M(t)^2 + \exp(-|t|/C) |x|_\infty)$$

and it follows that $M(0) \leq 1/2$ if $|x|_\infty$ is small enough.

#####

Using Lemma 4.1 and the Cauchy inequalities, we see that

$$(4.24) \|\phi_0''(x) - \phi_0''(0)\|_{\mathcal{X}(\ell_p^p, \ell_p^p)} = O(|x|_\infty)$$

Noticing that $v(t) = d_x \exp(t \nabla \phi_0(x) \cdot \partial_x)(x)(v(0))$ satisfies :

$$(4.25) \partial_t v(t) = \phi_0''(x(t)) v(t), \text{ where } x(t) = \exp(t \nabla \phi_0(x) \cdot \partial_x)(x),$$

using the arguments around the proof of (4.21)–(4.23), it is then easy to prove that

$$(4.26) \quad \|\mathbf{d}_x \exp(t \nabla \phi_0(x) \cdot \partial_x)(x)\|_{\mathcal{X}(\rho_p, \rho_p)} = O(1) \exp(-|t|/C), \quad t \leq 0$$

Let $\phi \sim \phi_0 + \phi_1 h + \phi_2 h^2 + \dots$,

be the (asymptotic) solution of the (complete) eiconal equation with

$$E \sim E_0 + E_1 h + E_2 h^2 + \dots :$$

$$(4.27) \quad V(x) - (1/2) |\nabla \phi(x)|_2^2 + h(\Delta \phi(x)/2 - E) = 0,$$

i.e.:

$$(E) \quad V(x) - (1/2) |\nabla \phi_0(x)|_2^2 = 0,$$

$$(T_1) \quad \nabla \phi_0(x) \cdot \partial_x \phi_1(x) = (\Delta \phi_0(x)/2) - E_0,$$

⋮

$$(T_k) \quad \nabla \phi_0(x) \cdot \partial_x \phi_k(x) =$$

$$= (\Delta \phi_{k-1}(x)/2) - (1/2) \sum_{j=1}^{k-1} \nabla \phi_j(x) \cdot \nabla \phi_{k-j}(x) - E_{k-1}.$$

Here recall that $E_0, \dots, E_{k-1}, \dots$ are defined by the condition that the r.h.s. of $(T_1), \dots, (T_k)$, vanish for $x = 0$.

Let us recall that $u = \exp(-\phi/h)$ is the approximate solution of :

$$-(h^2 \Delta/2) + V - hE(u) = 0$$

Proposition 4.2 :

There exists $r > 0$ independent of \mathcal{A} and of j such that

$$(4.28) \quad \|\nabla^2 \phi_j(x)\|_{\mathcal{X}(\rho_p, \rho_p)} = O_j(1)$$

for $|x|_\infty < r, 1 \leq p \leq \infty$.

Proof :

We recall from $[Sj]_1$ that we already know that $|\nabla \phi_j|_\infty = O_j(1)$ and

combining this with the Cauchy inequalities we obtain (4.28) in the special case when $\rho=1$. In the general case we have apparently to work with the Hessian directly, and we shall therefore take the Hessians of the r.h.s. of $(T_1), (T_2), \dots$.

Knowing (by Lemma (4.1)) that

$$|\langle \phi_0''(x), t \otimes s \rangle| = O(1) |t|_{p,\rho} \cdot |s|_{q,1/\rho}, \text{ with } (1/p) + (1/q) = 1,$$

we get by the Cauchy inequalities :

$$|\langle \nabla^2 \langle \phi_0''(x), t \otimes s \rangle, v \otimes \mu \rangle| = O(1) |t|_{p,\rho} \cdot |s|_{q,1/\rho} \cdot |v|_\infty \cdot |\mu|_\infty$$

and Lemma 1.2 of [Sj]₁⁴ implies that

$$\Delta \langle \phi_0''(x), t \otimes s \rangle = O(1) |t|_{p,\rho} \cdot |s|_{q,1/\rho}.$$

Hence

$$(4.29) \quad \|\Delta \phi_0''(x)\|_{\mathcal{L}(\ell_p^p, \ell_p^p)} = O(1).$$

We now differentiate (T_1) twice and get :

$$(4.30) \quad \nabla \phi_0(x) \cdot \partial_x (\nabla^2 \phi_1) + \phi_0'' \cdot \phi_1'' + \phi_1'' \cdot \phi_0'' \\ = (1/2) \Delta \phi_0'' - \nabla^3 \phi_0(x) \cdot L \nabla \phi_1(x)$$

where "L" means contraction of tensors :

$$\langle \nabla^3 \phi_0(x) \cdot L \nabla \phi_1(x), t \otimes s \rangle = \langle \nabla^3 \phi_0(x), \nabla \phi_1(x) \otimes t \otimes s \rangle.$$

By the Cauchy inequalities, Lemma (4.1) and the fact that $|\nabla \phi_1|_\infty = O(1)$,

we get that this expression is $O(1) |t|_{p,\rho} \cdot |s|_{q,1/\rho}$ and so we have :

$$(4.31) \quad \text{The norm in } \mathcal{L}(\ell_p^p) \text{ of } \nabla^3 \phi_0(x) \cdot L \nabla \phi_1(x) \text{ is } O(1).$$

Consider (4.30) along an integral curve $x = x(t) = \exp(t \nabla \phi_0 \cdot \partial_x)(x)$.

Let $\Phi(t,s)$ be the fundamental matrix for the corresponding problem:

$$\partial_t v(t) = - \phi_0''(x(t)) v(t),$$

⁴If A is a complex $N \times N$ matrix, then $|\text{Tr} A| \leq \|A\|_{\mathcal{L}(\ell_p^p, \ell_p^p)}$

that is the solution of :

$$(4.32) \quad \partial_t \Phi(t,s) = -\phi_0''(x(t))\Phi(t,s) ; \Phi(s,s) = 1$$

Then (see the proof of (4.26))

$$(4.33) \quad \|\Phi(t,s)\|_{\mathcal{L}(\ell^p)} = O(1) \exp(-(t-s)/C), \quad -\infty < s \leq t \leq 0 \\ = O(1) \exp(C|t-s|), \quad -\infty < t \leq s \leq 0$$

If B is a matrix, put :

$$\tilde{\Phi}(t,s)(B) = \Phi(t,s).B. {}^t\Phi(t,s).$$

Then $\tilde{\Phi}(s,s)B = B$ and $\tilde{\Phi}(t,s)$ is a solution of :

$$\partial_t \tilde{\Phi}(t,s)(B) + \phi_0''(x(t)) \tilde{\Phi}(t,s)(B) + \tilde{\Phi}(t,s)(B) \phi_0''(x(t)) = 0$$

(using that $\phi_0''(x(t))$ is symmetric). Notice that all non-trivial solutions of this equation explode as $t \rightarrow -\infty$. The non-exploding solution to (4.30) is then :

$$(4.34) \quad \phi_1''(x(t)) = \int_{-\infty}^t \tilde{\Phi}(t,s) ((1/2)\Delta\phi_0'' - \nabla^3\phi_0(x) L \nabla\phi_1)(x(s)) ds$$

which is (using (4.29), (4.31) and (4.33)) $O(1)$ in $\mathcal{L}(\ell^p)$.

Assume by induction that we have established (4.28) for $1 \leq j \leq k-1$.

Taking the Hessian of (T_k) we get :

$$(4.35) \quad \nabla\phi_0(x). \partial_x(\phi_k'') + \phi_0'' \cdot \phi_k'' + \phi_k'' \cdot \phi_0'' = \\ = -\nabla^3\phi_0(x) L \nabla\phi_k(x) + f_k''$$

where f_k is the r.h.s. of (T_k) .

Here $\|\phi_0'' L \phi_k'\|_{\mathcal{L}(\ell^p)} = O(1)$ by the same argument as before. Observe now that f_k'' contains terms of the form :

$$(1/2) \Delta\phi_{k-1}'', \phi_j'' \cdot \phi_{k-j}'', \phi_j''' L \phi_{k-j}'$$

which are all $O(1)$ in $\mathcal{L}(\ell^p)$. The solution of (4.35) is given by a formula analogous to (4.34) and it follows that (4.28) holds for $j = k$.

We shall next analyze the influence of a perturbation \mathcal{U} on V . Let us attach to the set \mathcal{A} the set \mathcal{B} defined again as a disjoint union over \mathbb{N} :

$$\mathcal{B} = \cup_m \mathcal{B}_m \quad \text{where } \mathcal{B}_m \subseteq \mathcal{V}_m \times \mathcal{A}_m$$

and let us assume that for all $(\mathcal{U}, \mathcal{V}, \rho)$ in \mathcal{B} , we have :

$$(4.36)_1 \quad |\nabla \mathcal{U}(x)|_{\rho, \infty} = O(1), \text{ uniformly in } x \text{ and } \mathcal{B}$$

and :

$$(4.36)_2 \quad (V_t, \rho) \text{ (with } V_t = V + t \mathcal{U}) \text{ belongs to } \mathcal{A} \text{ for all } t \in [0, 1]$$

(in particular we must have $\mathcal{U}(0) = 0, \mathcal{U}'(0) = 0, \|\mathcal{U}''(x)\|_{\mathcal{L}(\mathcal{E}_\rho^2)} = O(1)$ uniformly).

Let

$$\phi = \phi_t \sim \phi_{t,0} + \phi_{t,1} \hbar + \dots$$

be the phase associated to $V = V_t$.

Differentiating the eiconal equation with respect to t we get

$$(4.37) \quad (\nabla_x \phi_0, \partial_x) (\partial_t \phi_0) = \mathcal{U}$$

(here we take the notation $\phi_0(t, x) = \phi_{t,0}(x)$)

and hence :

$$(4.38) \quad (\partial_t \phi_0)(t, x) = \int_{-\infty}^0 \mathcal{U}(\exp(s \nabla_x \phi_0(t, x), \partial_x)(x)) ds .$$

We now observe that :

$$d(\mathcal{U}(\exp(s \nabla_x \phi_0(t, x), \partial_x)(x))) = d \mathcal{U} \cdot d(\exp(s \nabla_x \phi_0(t, x), \partial_x)(x)).$$

Using (4.5), (4.26) (with $p = 1$ and ρ replaced by $1/\rho$) and (4.36), we see that :

$$(4.39) \quad |\nabla_x \partial_t \phi_0|_{\infty, \rho} = O(1).$$

Assume by induction that we have proved that :

$$|\nabla_x \partial_t \phi_j|_{\infty, \rho} = O(1) \text{ for } 0 \leq j \leq k-1.$$

Differentiating T_k with respect to t , we get :

$$(4.40) \nabla_x \phi_0(t, x) \cdot \partial_x \partial_t \phi_k(t, x) = -\nabla \partial_t \phi_0(t, x) \cdot \nabla_x \phi_k + (\Delta \partial_t \phi_{k-1}(t, x)/2) - \sum_{j=1}^{k-1} \nabla_x \partial_t \phi_j(t, x) \cdot \nabla_x \phi_{k-j}(t, x) - \partial_t E_{k-1}(t).$$

The x -gradient of the l.h.s. is

$$\nabla_x \phi_0(t, x) \cdot \partial_x (\nabla_x \partial_t \phi_k(t, x)) + \phi_0''(t, x) \cdot \nabla_x \partial_t \phi_k(t, x)$$

and the x -gradient of the r.h.s. is a sum of terms of the form :

$$\alpha = \nabla_x^2(f) (\nabla_x g), \beta = \nabla_x^2(g) (\nabla_x f), \gamma = \Delta_x \nabla_x f$$

for various functions f and g satisfying

$$(4.41) \|\nabla_x f\|_{\infty, \rho}, \|\nabla_x g\|_{\infty, \rho}, \|\nabla_x^2 g\|_{\mathcal{L}(\ell_p^\infty)} = O(1).$$

(a) $f = \partial_t \phi_0(t, x)$, $g = \phi_k$ (the verification of (4.41) is obtained through (4.39), Proposition 3.1 in [Sj]₁, and Proposition (4.2)).

(b) $f = \partial_t \phi_{k-1}$ ((4.41) is satisfied by the induction assumption)

(c) $f = \partial_t \phi_j$, $g = \phi_{k-j}$ with $1 \leq j \leq k-1$.

We have by Cauchy (and (4.40)) :

$$\langle \nabla_x^2 f, v \otimes \mu \rangle = O(1) |v|_\infty |\mu|_{1, 1/\rho}$$

so

$$\|\nabla_x^2 f\|_{\mathcal{L}(\ell_p^\infty)} = O(1)$$

and hence $|\alpha|_{\infty, \rho} = O(1)$.

That $|\beta|_{\infty, \rho} = O(1)$ is immediate.

Finally we get $|\gamma|_{\infty, \rho} = O(1)$, by starting from $\langle \nabla_x f, v \rangle = O(1) |v|_{1, 1/\rho}$,

taking the Hessian, using the Cauchy inequalities :

$$\langle \nabla_x^2 \langle \nabla_x f, v \rangle, t \otimes s \rangle = O(1) |v|_{1, 1/\rho} |t|_\infty |s|_\infty$$

and finally Lemma 1.2 of [Sj]₁ to get :

$$\langle \nabla_x \Delta_x f, v \rangle = O(1) |v|_{1, 1/\rho}.$$

Then using the analog of (4.38) for $\nabla_x \partial_t \phi_k$ with \mathcal{U} replaced by the r.h.s. of (4.40) we get the control of $|\nabla_x \partial_t \phi_k|_{\infty, \rho}$. Then we have proved:

Proposition 4.3:

Under the assumptions (4.36), let ϕ_t be the phase associated to the perturbation $V_t = V + t \mathcal{U}$. Writing

$$\phi_t \sim \phi_{t,0} + \phi_{t,1} \hbar + \dots,$$

we have for every j , and uniformly for $(\mathcal{U}, V, \rho, t)$ in $\mathcal{B} \times [0, 1]$:

$$(4.42) \quad |\nabla_x \partial_t \phi_{t,j}|_{\infty, \rho} = O(\hbar) \text{ for } |x|_{\infty} \leq r.$$

We shall apply the above estimates to show the exponential convergence of the WKB ground state energy divided by the dimension, for a certain sequence of potentials : $V^{(m)}(x_1, \dots, x_m)$, $m = 1, 2, \dots$

Let us describe \mathcal{A} and \mathcal{B} in this case.

We start with this family $V^{(m)}$ defined for each m . For a given m , \mathcal{A}_m will be parametrized by n (with $1 \leq n \leq m-1$) : $\mathcal{A}_m = \cup_{1 \leq n \leq m-1} \mathcal{A}_m^n$.

For given n this is the set of pairs (V, ρ) where (using a notation introduced in the proof of Lemma 2.4)

$$(4.43) \quad V = (1-t) (V^{(n)} \oplus V^{(m-n)}) + t V^{(m)} \text{ for some } 0 \leq t \leq 1$$

and

(4.44) ρ belongs to $\mathcal{R}_m^n(\ell)$ defined as a set of applications on $\{1, \dots, m\}$ and satisfying⁵ :

$$\exp(-\ell) \leq \rho(j+1)/\rho(j) \leq \exp(\ell)$$

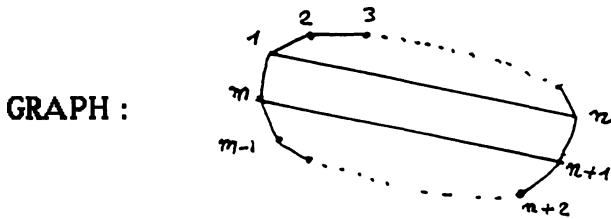
⁵ We can (if necessary) reduce ourselves to a smaller class with the additional assumption that $\rho(j) = 1$ for $j \geq n$.

(with the convention that if ρ is defined on $\{1, \dots, m\}$, $\rho(m+1) = \rho(1)$)

$$\exp(-\ell) \leq \rho(n)/\rho(1) \leq \exp(\ell)$$

$$\exp(-\ell) \leq \rho(m)/\rho(n+1) \leq \exp(\ell)$$

Notice that (4.44) gives bounds for $\rho(j)/\rho(k)$ when (j, k) is a pair of nearest neighbors in the graph :



Similarly the set \mathfrak{B} is defined by describing \mathfrak{B}_m as $\cup_n \mathfrak{B}_m^n$ where :

$$(4.45) \quad \mathfrak{B}_m^n \text{ is the set } \{ \mathcal{U}_n^m \times \mathcal{A}_m^n, \text{ with } \mathcal{U}_n^m = (V^{(m)} - V^{(n)}) \tilde{\oplus} V^{(m-n)} \}$$

Let us assume that, for a suitable ℓ , the assumptions of Proposition (4.3) are satisfied for the set \mathfrak{B} associated to the sequence $V^{(m)}$ (we shall give in §6 examples where this is true). Then if $\phi^{(m)}$ denotes the phase associated to $V^{(m)}$ we obtain by integrating

(4.42) with respect to t :

$$(4.46) \quad |\nabla(\phi_k^{(m+\rho)} - \phi_k^{(m)} \tilde{\oplus} \phi_k^{(\rho)})|_{\infty, \rho} = O(1), \quad |x| < r.$$

We choose $\rho(s) = \exp(\ell \min(s, m+1-s))$ (for $1 \leq s \leq m+1$) and $\rho = 1$ for $s \geq m+1$. We add one more assumption :

$$(4.47) \quad \text{For every } m, V^{(m)} \text{ is invariant under cyclic permutations of the}$$

coordinates : $V^{(m)}(x_m, x_1, \dots, x_{m-1}) = V^{(m)}(x_1, \dots, x_m)$.

Then $\phi^{(m)}$ will have the same property. Let

$hE(m) \sim h(E_0(m) + E_1(m)h + \dots)$

be the WKB ground state of $-(\hbar^2/2)\Delta + V^{(m)}$.

We recall that we have seen just before the Proposition (4.2) the following equality :

$$(4.48) E_k(m) = (\Delta \phi_k^{(m)}(0)/2) - (1/2) \sum_{j=1}^k \nabla \phi_j^{(m)}(0) \cdot \nabla \phi_{k+1-j}^{(m)}(0)$$

and using the cyclic invariance of $\phi^{(m)}$ we get for any $s \in \{1, \dots, m\}$:

$$(4.49) (E_k(m)/m) = \partial_{x_s}^2 \phi_k^{(m)}(0) - (1/2) \sum_{j=1}^k \partial_{x_s} \phi_j^{(m)}(0) \cdot \partial_{x_s} \phi_{k+1-j}^{(m)}(0).$$

Choosing s with $|s - (m/2)| \leq 1$, we obtain from (4.46) that :

$$\partial_{x_s} \phi_k^{(m+p)}(x_1, \dots, x_{m+p}) - \partial_{x_s} \phi_k^{(m)}(x_1, \dots, x_m) = O(\exp(-\ell m/2))$$

By Cauchy's inequality, we can replace ∂_{x_s} by $\partial_{x_s}^2$. Using these estimates with (4.49), we get :

$$(4.50) (E_k(m+p)/(m+p)) - (E_k(m)/m) = O_k(\exp(-\ell m/2)).$$

which gives for each k the exponential convergence of the $E_k(m)/m$ as m tends to ∞ .

To summarize, we have proved the

Theorem 4.4

If the sequence of potentials $V^{(m)}$ satisfies uniformly (4.1), (4.2), (4.3), (4.4) and (4.36) for the family of $\rho \in \mathcal{R}_m^n(\ell)$ introduced in (4.44)⁶, then the first eigenvalue of the Schrödinger operator : $-(\hbar^2/2) \Delta_m + V^{(m)}$

⁶ More precisely, we have associated to the sequence $V^{(m)}$ and to a set of weights $\mathcal{R}_m^n(\ell)$ a set \mathcal{A} and a set \mathcal{B} . The exact assumption is that we can find ℓ s.t. all the assumptions concerning \mathcal{A} and \mathcal{B} are satisfied.

admits an asymptotic expansion of the form : $h \sum_{k \geq 0} E_k(m) \cdot h^k$.

The sequence $E_k(m)/m$ is convergent to a limit E_k^∞ and we have the following inequality :

For all k , there exists C_k s.t.

$$(4.51) |E_k^\infty - (E_k(m)/m)| \leq C_k \exp(-\ell m/2).$$

§5 Comparison between the Dirichlet problem in a box and the global problem

§5.1 Introduction :

In $[Sj]_1$, the semi-classical study of the fundamental level of the Dirichlet realization in a sufficiently small box was achieved. The validity of the results was subsequently extended in $[Sj]_2$. We are here in the apparently very simple case of a one well problem, and it is natural to think (but difficult to control with respect to m) that the first eigenvalue of the Dirichlet problem in a box containing the unique minimum of the potential will be in the semi-classical limit quite near of the first eigenvalue of the global problem in \mathbb{R}^m . We shall prove, following essentially the ideas of $[Sj]_1$ § 5-6, that it is effectively the case under the restrictive condition on the dimension that :

$$(5.1.1) m = O(h^{-N_0}) \text{ for some fixed } N_0.$$

This is naturally not completely satisfactory for our purpose but we shall see how to circumvent this problem in §6. In the two next sections, we shall construct as a preliminary step for a procedure of localization of

estimates a suitable family of boxes covering \mathbb{R}^m . The idea behind this construction is to compare (more precisely to minorize) by a suitable translation the potential in any box of the family and the potential in a box centered at the minimum of the potential.

§5.2 Case of a quadratic potential :

Let us consider

$$V(x) = (1/2) \langle V''(0)x, x \rangle$$

with (see the stronger assumptions we make in §4)

$$(5.2.1) V''(0) = D + A, \text{ with } D \text{ diagonal,}$$

$$\|A\|_{\mathcal{L}(\ell^\infty)} \leq r_1 < r_0 \leq \lambda_{\min}(D) \leq \lambda_{\sup}(D) \leq C_0$$

r_1, r_0, C_0 are fixed and independent of the dimension m .

These assumptions were introduced in $[Sj]_2$.

Then we know from $[Sj]_2$ (and we have already used in (4.7)₁) that

$$(5.2.2) V''(0)^{1/2} = \tilde{D} + \tilde{A}, \text{ with } \tilde{D} \text{ diagonal,}$$

$$\|\tilde{A}\|_{\mathcal{L}(\ell^\infty)} \leq \tilde{r}_1 < \tilde{r}_0 \leq \lambda_{\min}(\tilde{D}) \leq \lambda_{\sup}(\tilde{D}) \leq \tilde{C}_0$$

$\tilde{r}_1, \tilde{r}_0, \tilde{C}_0$ are fixed and independent of the dimension m .

It will be easier to work in the Morse coordinates :

$$(5.2.3) y = V''(0)^{1/2} x$$

since we get in the new coordinates :

$$(5.2.4) V(x) = y^2 / 2.$$

As in $[Sj]_1$ §5,6, we consider then the following family of boxes, which depends on 2 parameters C and ϵ . The center of the box Ω_ρ is $\rho = (\rho_1, \dots, \rho_m)$ and $\Omega_\rho = I_{\rho_1} \times \dots \times I_{\rho_m}$ in the new coordinates. Here for each j , we have

$\rho_j = 0$ or $\rho_j \geq C\varepsilon$, and in the first case $I_{\rho_j} = [-C\varepsilon, C\varepsilon]$ while in the second case $I_{\rho_j} = [\rho_j - \varepsilon, \rho_j + \varepsilon]$. Here $C \geq 1$, $\varepsilon > 0$.

Using (5.2.4) it is easy to see that :

$$(5.2.5) \quad V(x) - V(x - \rho) \geq (1 - \eta(C)) V(\rho), \quad x \in \Omega_\rho,$$

where $\eta(C)$ is independent of ε and tends to 0 when C tends to ∞ .

The Ω_ρ are somewhat distorted boxes, but since

$$(5.2.7) \quad |y|_\rho \sim |x|_\rho, \quad 1 \leq \rho \leq \infty,$$

the ℓ^∞ -diameter of Ω_ρ is $O(\varepsilon)$ when C is fixed.

§5.3 The general case.

Let $V : \mathbb{R}^m \rightarrow \mathbb{R}$ be smooth with :

$$(5.3.1) \quad V(0) = 0, \quad V'(0) = 0 \quad \text{and} \quad V''(0) \text{ satisfying (5.2.1).}$$

$$(5.3.2) \quad \langle V''(x), t_1 \otimes t_2 \rangle = O(1) |t_1|_{p_1} |t_2|_{p_2}$$

uniformly in x, t_1, t_2 and for all p_1, p_2 s.t. $1 = 1/p_1 + 1/p_2$.

$$(5.3.3) \quad \langle V'''(x), t_1 \otimes t_2 \otimes t_3 \rangle = O(1) |t_1|_{p_1} |t_2|_{p_2} |t_3|_{p_3}$$

uniformly in x, t_1, t_2, t_3 and for all p_1, p_2, p_3 s.t. $1 = 1/p_1 + 1/p_2 + 1/p_3$.

We write

$$(5.3.4) \quad V(x) = V_0(x) + \mathcal{L}(x) \quad \text{with} \quad V_0(x) = (1/2) \langle V''(0)x, x \rangle.$$

So we have the property (5.2.6) for V_0 :

$$(5.3.5) \quad V_0(x) - V_0(x - \rho) \geq (1 - \eta(C)) V_0(\rho), \quad x \in \Omega_\rho,$$

and \mathcal{L} vanishes to the third order at 0 and satisfies (5.3.3).

Let $\rho + x \in \Omega_\rho$ (so that $x \in \Omega_0$). Then :

$$\mathcal{L}(\rho + x) - \mathcal{L}(x) = \mathcal{L}(\rho) - \mathcal{L}(0) + \langle \nabla \mathcal{L}(\rho) - \nabla \mathcal{L}(0), x \rangle$$

$$\begin{aligned}
 & + \int_0^1 (1-t) \langle \nabla^2 \varphi(\rho + tx) - \nabla^2 \varphi(tx), x \otimes x \rangle dt \\
 = & \varphi(\rho) + \int_0^1 \int_0^1 \langle \nabla^3 \varphi(tsp), \rho \otimes \rho \otimes x \rangle t dt ds \\
 & + \int_0^1 \int_0^1 (1-t) \langle \nabla^3 \varphi(sp + tx), \rho \otimes x \otimes x \rangle dt ds
 \end{aligned}$$

$$(5.3.6) \quad \varphi(\rho + x) - \varphi(x) = \varphi(\rho) + O(1)|x|_\infty |\rho|_2^2 + O(1)|x|_\infty^2 |\rho|_1.$$

For the particular choices of ρ which are allowed, we see that

$$(5.3.7) \quad C\varepsilon |\rho|_1 \leq \tilde{C}_0 |\rho|_2^2$$

where C and ε appear in the choice of Ω_ρ and \tilde{C}_0 only depends on the constants appearing in (5.2.1) (see 5.2.7)).

On the other hand

$$(5.3.8) \quad |x|_\infty = O(C\varepsilon)$$

so, with a new constant (with the same properties as the first one), we get :

$$(5.3.9) \quad |x|_\infty |\rho|_1 \leq \tilde{C}_0 |\rho|_2^2$$

Finally we get from (5.3.6) – (5.3.9) that :

$$(5.3.10) \quad \varphi(\rho + x) - \varphi(x) = \varphi(\rho) + O(1) C\varepsilon |\rho|_2^2$$

If we combine with the properties of V_0 , we get for each x in Ω_ρ :

$$(5.3.11) \quad V(x) - V(x - \rho) \geq V(\rho) - \eta(C) V_0(\rho) - O(1) C\varepsilon |\rho|_2^2.$$

For every $\delta > 0$, we get by choosing first C sufficiently large and then ε sufficiently small :

$$(5.3.12) \quad V(x) - V(x - \rho) \geq V(\rho) - \delta |\rho|_2^2, \text{ for } x \in \Omega_\rho.$$

(Here we have used (5.3.2) for the first time).

If we have the additional property that :

$$(5.3.13) \quad V''(x) \geq \omega I > 0,$$

there is a choice of ε and C in the construction of the ball s.t., for some $\delta_0 > 0$, we have :

$$(5.3.14) \quad V(x) - V(x-\rho) \geq \delta_0 |\rho|_2^2, \text{ for } x \in \Omega_\rho.$$

(compare this estimate with (6.2) in [Sj]₁)

§5.4 Statement of the result and end of the proof :

Theorem 5.4.1

Let V satisfy (5.2.1), (5.3.1)–(5.3.3), (5.3.13) and

(5.4.1) V extends holomorphically to $\{x \in \mathbb{C}^m; |x|_\infty < r_0\}$ and $|\nabla V|_\infty = O(1)$ in this polydisc.

We assume that the condition $m = O(h^{-N_0})$ is satisfied. Then the first eigenvalue of the Schrödinger equation in \mathbb{R}^m $\lambda_1(m, h)$ is of the form $hE(m) + O(h^\infty)$ (where $hE(m)$ is the WKB eigenvalue constructed in [Sj]₂ , see also §4).

Sketch of the proof

This is essentially the same proof as in [Sj]₁ using the improvements in [Sj]₂ and the new construction of boxes we give in sections 5.1–5.3. Let us recall some of the steps.

We choose $\varepsilon > 0$ so that $C\varepsilon < r_0$. Let us first consider the Dirichlet realization P_{Ω_0} of $-(h^2\Delta/2) + V$ in the "twisted" box Ω_0 . In view of (5.4.1), we can construct as in [Sj]₂ (see our section 4) a WKB-candidate $hE(h)$ for the lowest eigenvalue of P_{Ω_0} with :

$$(5.4.2) \quad E(h) \sim E_0 + E_1 h + \dots, \quad E_0 \sim m, \quad E_j = O_j(m)$$

and modifying $E(h)$ by $O(mh^\infty)$ we also know from the arguments of $[Sj]_2$ that $hE(h)$ is exactly equal to the lowest eigenvalue of P_{Ω_0} , when h is small enough. The only slightly new point here is that Ω_0 is not exactly a ℓ^∞ -ball in the x -coordinates. However, it is enough to notice according to (5.2.7) that

$$(5.4.3) \quad B(0, C\epsilon/C_1) \subset \Omega_0 \subset B(0, C_1 C\epsilon)$$

with $B(x_0, r) = \{x \in \mathbb{R}^n; |x - x_0| < r\}$.

Let us now observe that by monotonicity we have :

$$(5.4.4) \quad \lambda_1(m, h) \leq hE(h).$$

In order to get a lower bound, we follow the general strategy of $[Sj]_1$ (sections 5, 6) and start by establishing some exponentially weighted estimates in Ω_0 . Lemma 5.1 of $[Sj]_1$ remains valid in the present context and we conclude that if $\tilde{V} = V - \sum x_j^{2M}$, and if $h\tilde{E}$ is the lowest eigenvalue of the Dirichlet realization of $-(h^2\Delta/2) + \tilde{V}$ in Ω_0 , then

$$(5.4.5) \quad E - \tilde{E} = O(1) m \cdot h^{M-1}.$$

As in the end of section 5 of $[Sj]_1$ we then obtain the estimate

$$(5.4.6) \quad (hE - O(1)mh^{M-1})\|u\|^2 \leq (\exp(\psi/h)(-(h^2\Delta/2)+V) \exp(-\psi/h)u|u),$$

for each $u \in C_0^\infty(\Omega_0)$, provided that ψ is a real valued smooth function, defined on Ω_0 with

$$(5.4.7) \quad (1/2) |\nabla\psi(x)|^2 \leq \sum_{j=1}^m x_j^{2M}, \quad x \in \Omega_0.$$

Replacing u by $\exp(\psi/h)u$, we can rewrite (5.4.6) as

$$(5.4.8) \quad (hE - O(1)mh^{M-1})\|\exp(\psi/h)u\|^2 \leq (\exp(\psi/h)(-(h^2\Delta/2)+V) u|\exp(\psi/h)u), \text{ for each } u \in C_0^\infty(\Omega_0).$$

Using now (5.3.14), we deduce from (5.4.8)

(5.4.9) $(hE - O(1)mh^{M-1}) \|\exp(\psi/h)u\|^2$
 $\leq (\exp(\psi/h)(-h^2\Delta/2 + V)u) \exp(\psi/h)u$, for each $u \in C_0^\infty(\Omega_\rho)$, provided
 that ψ is a real valued smooth function, defined on Ω_ρ with

$$(5.4.10) \quad (1/2) |\nabla\psi(x)|^2 \leq \sum_{j=1}^m (x_j - \rho_j)^{2M}, \quad x \in \Omega_\rho.$$

Then we have just to control the patching procedure which appears in the estimate (6.18) in [Sj]₁. The patching procedure is based on a resolution of the identity. We just take the same one but in the y variables. The only new problem occurs in the control of the commutators.

For that, we only need to observe that (with the notations of § 5.2), if we introduce cutoff functions of the form

$$(5.4.11) \quad \chi(x) = \prod_1^m \chi_j(y_j),$$

where :

$$(5.4.12) \quad |\chi_j(t)| \leq 1$$

and

$$(5.4.13) \quad |\chi_j'(t)| + |\chi_j''(t)| \leq D$$

(where D is independent of j),

then :

$$(5.4.14) \quad |\nabla_x \chi(x)|_\infty \leq C(D)$$

$$(5.4.15) \quad |\Delta_x \chi(x)| \leq C(D) m^{3.7}$$

Let us prove for instance (5.4.14) :

$$\partial_{x_v} \chi = \sum_1^m \chi_1(y_1) \dots \chi_{k-1}(y_{k-1}) (\partial_{x_v} (\chi_k(y_k)) \chi_{k+1}(y_{k+1}) \dots \chi_m(y_m))$$

$$\text{with } \partial_{x_v} (\chi_k(y_k)) = \chi_k'(y_k) (\partial_{x_v} (y_k)) = (V''(0))^{1/2}_{kv} \chi_k'(y_k).$$

⁷ In fact using lemma 1.2 in [Sj]₁ we can get O(m) but this improvement is of no use here.

This gives us :

$$\begin{aligned} \partial_{x_v} \chi &= \sum_{k=1}^m (V''(0)^{1/2})_{kv} \chi_1(y_1) \dots \chi_{k-1}(y_{k-1}) \chi_k' \chi_{k+1}(y_{k+1}) \dots \chi_m(y_m) \\ &= \sum_{k=1}^m (V''(0)^{1/2})_{kv} t_k(y) \end{aligned}$$

with $t_k(y) = \chi_1(y_1) \dots \chi_{k-1}(y_{k-1}) \chi_k' \chi_{k+1}(y_{k+1}) \dots \chi_m(y_m)$.

According to (5.4.12) and (5.4.13), $(t_k(y))_k$ is in a bounded ball of ℓ^∞ and using (5.2.2), we get (5.4.14).

The control of cut off terms occurs in the proof in §6 of [Sj]₁ only in passing from (6.18) to (6.19). These terms are multiplied by an exponentially small (w.r.to h) term and as in [Sj]₁ we get

$$\begin{aligned} (5.4.15) \quad & (hE - O(1)mh^{M-1})(1 + O(\exp(-1/Ch))) \|u\|^2 \\ & \leq \int (1 + O(\exp(-1/Ch))) (-h^2 \Delta/2 + V) u \, dx \\ & \quad + \int (O(\exp(-1/Ch)) |u| |\nabla u|_2 \, dx \end{aligned}$$

Since $V \geq 0$, we have

$$(h^2/2) \int |\nabla u|_2^2 \, dx \leq \int (-h^2 \Delta/2 + V) u \, dx,$$

so we end up with

$$\begin{aligned} (5.4.16) \quad & (hE - O(1)mh^{M-1}) \|u\|^2 \\ & \leq \int (1 + O(\exp(-1/Ch))) (-h^2 \Delta/2 + V) u \, dx. \end{aligned}$$

Taking for u a sequence of truncations of the first eigenfunction, we get in the limit : $hE - O(1)mh^{M-1} \leq (1 + O(\exp(-1/\tilde{C}h))) \lambda_1(m, h)$

and combining with (5.4.4) :

$$(5.4.17) \quad hE - O(1)mh^{M-1} \leq \lambda_1(m, h) \leq hE.$$

§6. Complete study of the model for $v < 1/4$. proof of Theorem 1.1.

We return in this section to the initial conventions to work with

$$-\hbar^2 \Delta + V.$$

(Note that it is easy to go from one convention to the other by a change of

$$\hbar : \tilde{\hbar} = \hbar/\sqrt{2}).$$

§6.1 Summary of the different steps :

As we have seen in Theorem 5.4.1 :

$$(6.1.1) \lambda_1(m; \hbar) \sim \hbar \sum_{j \geq 0} \Lambda_j(m) \hbar^j \quad \text{if } m = O(\hbar^{-N_0})$$

$$(\text{with } \Lambda_j(m) = E_j(m) \cdot 2^{-(j+1)/2}).$$

But we have seen in §2, that :

$$(6.1.2) |(\lambda_1(m; \hbar)/m) - \text{Lim}_{m \rightarrow \infty} (\lambda_1(m; \hbar)/m)| \leq C\hbar/m$$

Taking $m = \hbar^{-M}$, we get (using Theorem 4.4) the existence of a sequence

Λ_j s.t. :

$$(6.1.3) | \hbar (\sum_{M \geq j \geq 0} \Lambda_j \cdot \hbar^j) - \text{Lim}_{m \rightarrow \infty} (\lambda_1(m; \hbar)/m) | \leq C_M \cdot \hbar^M$$

as \hbar tends to 0, where :

$$(6.1.4) \Lambda_j = \text{Lim}_{m \rightarrow \infty} (\Lambda_j(m)/m)$$

Of course we have to verify that all the conditions of the different theorems we use are satisfied for Example 2.6.

But before let us give a weaker result which can be obtained easier and some explicit computations on the harmonic approximation permitting to determine Λ_0 .

Lemma 6.1.1

There exists a constant C such that, for all $h \in]0, h_0]$ and all $m \geq 1$, we have :

$$(6.1.5) \quad 0 \leq \lambda_1(m; h, \nu) - (h/2) \sum_{k=0}^{m-1} (\sqrt{\omega_k(m; \nu)}) \leq C m \cdot h^2$$

where the $\omega_k(m; \nu)$ are given by :

$$(6.1.6) \quad \omega_k(m; \nu) = 1 - 4\nu \cos^2(\pi k/m) ; k = 0, 1, \dots, m-1$$

Proof

The $(\omega_k(m; \nu)/2)$ are just the eigenvalues of the Hessian of the potential $V^{(m)}$ at 0. An easy computation (cf [Ka]₂) gives (6.1.5) (see § 6.2).

The minoration is just that in this case the potential $V^{(m)}$ dominates everywhere its quadratic approximation in view of

$$(6.1.7) \quad -\log \operatorname{ch} s \geq -s^2/2$$

so we get immediately the lower bound in (6.1.5).

For the upper bound, it is sufficient to use the eigenfunction corresponding to the harmonic approximation and to estimate carefully the error using the inequality :

$$(6.1.8) \quad |-\log \operatorname{ch} s + s^2/2| \leq C s^4$$

The details are for example computed in [Ka]₂ (p.293-294).

We just give now for completeness some of the computations relative to the harmonic oscillator.

The harmonic approximation at 0 is given in the case of Example (2.6) by the potential :

$$(6.1.9) \quad Q_m(x) = (1/4) \sum_{k=1}^m x_k^2 - (\nu/4) (\sum_{k=1}^m (x_k + x_{k+1}))^2$$

Let us now remark that :

$$(6.1.10) \text{Lim}_{m \rightarrow \infty} [(1/2m) \sum_{k=0}^{m-1} (\sqrt{\omega_k})] = \\ = (1/2\pi) \int_0^\pi \sqrt{1-4v \cdot \cos^2 \theta} \, d\theta$$

Using directly the Mac-Laurin formula (cf for example [Di], p.302) or Fourier series and Parseval, we get :

$$(6.1.11) |[\text{Lim}_{m \rightarrow \infty} [(1/2m) \sum_{k=0}^{m-1} \sqrt{\omega_k}]] - \\ - [(1/2\pi) \int_0^\pi \sqrt{1-4v \cdot \cos^2 \theta} \, d\theta]| \leq [(Cr/m)^{2(r/m)}]^m$$

for all r. By choosing correctly r (=αm) we get the exponential convergence which was proved in the general case in §4. We have used here the π-periodicity and the analyticity of the function $\theta \rightarrow \sqrt{1-4v \cdot \cos^2 \theta}$.

§6.2 Verification of the conditions for the Example 2.6

We shall verify the following properties for the potential $V = V^{(m)}$ which is given by

$$(6.2.1) V^{(m)}(x) = (1/4) \sum_{k=1}^m x_k^2 - \sum_{k=1}^m \log \text{ch}(\sqrt{v/2} (x_k + x_{k+1})).$$

$$(6.2.2) V \text{ is holomorphic in } B_\infty(0,1) \text{ with } |\nabla V(x)|_\infty = O(1),$$

$$(6.2.3) V(0) = 0, V'(0) = 0,$$

$$(6.2.4) V''(0) = D + A, \text{ where } D \text{ is diagonal (positive definite) and}$$

$$\|A\|_{\mathcal{L}(\ell_p^m, \ell_p^m)} \leq r_1 < r_0 \leq \lambda_{\min}(D) \text{ for all } p \text{ s.t. } 1 \leq p \leq \infty \text{ and for all } \rho \text{ with :}$$

$$(*) \exp(-\ell) \leq \rho(j+1)/\rho(j) \leq \exp(\ell).$$

$$(6.2.5) \|\nabla^2 V\|_{\mathcal{L}(\ell_p^m, \ell_p^m)} = O(1)$$

uniformly in $B_\infty(0,1)$ for ρ satisfying (*).

$$(6.2.6) V^{(m)''}(x) \geq ((1-4v)/2) \cdot I_m$$

and in particular V is convex for $v < 1/4$.

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

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

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

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

$$|\nabla \mathcal{W}_n^m|_{e_p^\infty} = O(1) \text{ in a complex ball } B(0,1).$$

(6.2.8) $V^{(m)}$ and more generally $(1-t) (V^{(n)} \tilde{\oplus} V^{(m-n)}) + t V^{(m)}$ for $0 \leq t \leq 1$ satisfy (6.2.2)–(6.2.4) uniformly for the ρ satisfying (*) and

(**) (more generally (*) and

$$\exp(-\ell) \leq \rho(n)/\rho(1) \leq \exp(\ell)$$

(***)

$$\exp(-\ell) \leq \rho(m)/\rho(n+1) \leq \exp(\ell)$$

$$(6.2.9) \langle V''(x), t_1 \otimes t_2 \rangle = O(1) |t_1|_{p_1} |t_2|_{p_2}$$

uniformly in x, t_1, t_2 and for all p_1, p_2 s.t. $1 = 1/p_1 + 1/p_2$.

$$(6.2.10) \langle V'''(x), t_1 \otimes t_2 \otimes t_3 \rangle = O(1) |t_1|_{p_1} |t_2|_{p_2} |t_3|_{p_3}$$

uniformly in x, t_1, t_2, t_3 and for all p_1, p_2, p_3 s.t. $1 = 1/p_1 + 1/p_2 + 1/p_3$.

(6.2.11) For every m , $V^{(m)}$ is invariant under cyclic permutations of the coordinates : $V^{(m)}(x_m, x_1, \dots, x_{m-1}) = V^{(m)}(x_1, \dots, x_m)$.

The verification of (6.2.2) is easy. We just observe (always with the convention that $x_{m+1} = x_1$) that :

$$(6.2.12) \partial_{x_j} V^{(m)}(x) = \\ = (x_j/2) - \sqrt{v/2} \operatorname{th}(\sqrt{v/2} (x_j + x_{j+1})) - \sqrt{v/2} \operatorname{th}(\sqrt{v/2} (x_j + x_{j-1}))$$

and that if $|x|_\infty \leq 1$,

$$|\sqrt{v/2} (x_j + x_{j+1})| \leq \sqrt{2v} \leq \sqrt{1/2} < \pi/2$$

which implies that $\partial_{x_i} V^{(m)}(x)$ is bounded independently of m .

Let us observe for future use that :

$$(6.2.13) \quad (\partial_{x_i}^2 V^{(m)})(x) = \\ = ((1/2) - v) + (v/2)[\text{th}^2(\sqrt{v/2} (x_j + x_{j+1})) + \text{th}^2(\sqrt{v/2} (x_j + x_{j-1}))]$$

$$(6.2.14) \quad \partial_{x_i} \partial_{x_{i+1}} V^{(m)}(x) = \\ = -v/2 (1 - \text{th}^2(\sqrt{v/2} (x_j + x_{j+1}))) = -v/(2 \text{ch}^2(\sqrt{v/2} (x_j + x_{j+1})))$$

$$(6.2.15) \quad \partial_{x_i} \partial_{x_k} V^{(m)}(x) = 0 \quad \text{if } |j-k| \neq 0, -1, +1 \text{ modulo } m.$$

For (6.2.4) we deduce from (6.2.13) :

$$(6.2.16) \quad D = ((1/2) - v) I_m$$

where I_m is the identity in \mathbb{R}^m , so we have :

$$(6.2.17) \quad r_0 = \lambda_{\min}(D) = ((1/2) - v).$$

If we denote by τ the operator of translation (by 1) on \mathbb{R}^m defined by:

$(\tau x)_i = x_{i-1}$, we can write :

$$(6.2.18) \quad A = - (v/2) (\tau + \tau^{-1})$$

The eigenvalues of A are easily computed as $-v \cdot \cos(2\pi k/m)$ for $k = 0, 1, \dots, m-1$.

It is then easy to verify that for ρ satisfying to (*):

$$(6.2.19) \quad \|A\|_{\mathcal{L}(e_\rho^0, e_\rho^0)} \leq v \cdot \exp(\rho)$$

If $v < 1/4$, we observe that one can choose ρ such that :

$$(6.2.20) \quad r_1 = v \cdot \exp(\rho) < ((1/2) - v)$$

and we shall make this choice now.

The proof of (6.2.5) is immediate if we observe that all the second derivatives

are bounded and that we have (6.2.15). (6.2.6) is a consequence of (6.2.13)–(6.2.15). Let us now verify (6.2.7). We just observe (with the notation of §2) that :

$$\begin{aligned} \mathcal{U}_n^m &= W(x_m, x_1) + W(x_n, x_{n+1}) - W(x_n, x_1) - W(x_m, x_{n+1}) \\ &= \log \operatorname{ch}(\sqrt{\nu/2} (x_m + x_1)) + \log \operatorname{ch}(\sqrt{\nu/2} (x_n + x_{n+1})) \\ &\quad - \log \operatorname{ch}(\sqrt{\nu/2} (x_n + x_1)) - \log \operatorname{ch}(\sqrt{\nu/2} (x_m + x_{n+1})) \end{aligned}$$

The only j for which $\partial_{x_j} \mathcal{U}_n^m$ are not 0 are $j = 1, n, n+1, m$ and one has for each of these terms :

$$|\partial_{x_j} \mathcal{U}_n^m(x)| \leq 4 \sqrt{\nu/2} \operatorname{Sup}_{\tau \in \mathbb{C}, |\tau| \leq 1} (\operatorname{th}(\sqrt{2\nu} \tau))$$

for $x \in \mathbb{C}^m, |x|_\infty \leq 1$.

As in the proof of (6.2.12), $\operatorname{Sup}_{\tau \in \mathbb{C}, |\tau| \leq 1} (\operatorname{th}(\sqrt{2\nu} \tau))$ is finite.

According to the (**), the property (6.2.7) is clear.

Let us verify now (6.2.8). We first observe that :

$$\begin{aligned} D_t^{(m)} &= (1-t) D^{(n)} \otimes D^{(m-n)} + t A^{(m)} \quad \text{and :} \\ A_t^{(m)} &= (1-t) A^{(n)} \otimes A^{(m-n)} + t A^{(m)}. \end{aligned}$$

All the properties we need are stable by arithmetical means, so it is sufficient to treat the case $(V^{(n)} \oplus V^{(m-n)})$ 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 $\|A\| \leq \nu \cdot \exp(\kappa)$.

If $\nu < 1/4$, it is easy to choose $\kappa > 0$ s.t :

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

(6.2.9) and (6.2.10) are then easy to verify by using (6.2.13)–(6.2.15).

Finally, (6.2.11) is clear from the definition.

Références

[Ag] S.Agmon

Lectures on exponential decay of solutions of second order elliptic equations,
Math. Notes, t.29, Princeton University Press.

[Bra–Li] H.J.Brascamp, E.Lieb :

On extensions of the Brunn–Minkovski and Prékopa–Leindler Theorems,
including inequalities for Log concave functions, and with an application to
diffusion equation

Journal of functional analysis 22 (1976), pp.366–389

[Bru–He] M.Brunaud, B.Helffer :

Un problème de double puits provenant de la théorie statistico–mécanique
des changements de phase (ou relecture d’un cours
de M.Kac), Preprint de l’ENS (Mars 1991).

[Di] J.Dieudonné :

Calcul infinitésimal, Hermann; collection méthodes

[Gl–Ja] J.Glimm, A.Jaffe

Quantum Physics (second edition), A functional integral point of view.
Springer Verlag

[Ha] E.M.Harrell,

On the rate of asymptotic eigenvalue degeneracy
Comm.in Math. Phys., t.75, 1980, p.239–261

[He] B.Helffer :

Décroissance exponentielle des fonctions propres de l'opérateur de Kac : cas de la dimension >1 . Manuscrit, Mars 1991

[He-Sj] B.Helffer, J.Sjostrand :

[1] Multiple wells in the semi-classical limit I

Comm. in PDE, 9(4), 337-408 (1984)

[2] Puits multiples en limite semi-classique II

Interaction moléculaire. Symétries. Perturbation

Ann.Inst. Henri Poincaré Vol.42, n°2, 1985, p.127-212

[3] Multiple wells in the semi-classical limit III

Math.Nachrichte 124 (1985) p.263-313

[4] Analyse semi-classique pour l'équation de Harper

Mémoire de la SMF n°34; Tome 116, Fasc.4 (1988)

[Ka] M.Kac

[1] Statistical mechanics of some one-dimensional systems

Studies in mathematical analysis and related topics : essays in honor of Georges Polya (Stanford Univ. Press, Stanford, California 1962), p.165-169

[2] Mathematical mechanisms of phase transitions

Brandeis lectures (1966), Gordon and Breach, New York

[Ka-Th] M.Kac, C.J.Thomson

Phase transition and eigenvalue degeneracy of a one dimensional anharmonic oscillator

Studies in Applied Mathematics 48 (1969) 257–264

[Ki–Si] W.Kirsch, B.Simon :

Comparison theorems for the gap of Schrödinger operators

JFA , Vol.75, n°2, Dec.1987, p.396–410

[PPW] L.E. Payne, G.Polya, H.F.Weinberger :

On the ratio of consecutive eigenvalues,

Journal of Math. and Physics, 35, n°3 (Oct.56), pp.289–298

[Ru] D.Ruelle :

Statistical mechanics

Math. physics monograph series, W.A.Benjamin, Inc. 1969

[Si] B.Simon

[1] Instantons, double wells and large deviations

Bull.AMS., t.8, 1983 p.323–326

[2] Semi–classical analysis of low lying eigenvalues I

Ann. Inst. Poincaré, t.38, 1983, p.295–307

[3] Semi–classical analysis of low lying eigenvalues

II tunneling, Ann. of Math. 120, p.89–118 (1984)

[SWYY] I.M.Singer, B.Wong, Shing–Tung Yau, Stephen S.–T.Yau :

An estimate of the gap of the first two eigenvalues in the Schrödinger operator.

Ann. d. Scuola Norm. Sup. di Pisa , Série IV Vol. XII,2, p.319–333

[Sj] J.Sjöstrand :

[1] Potential wells in high dimensions I

(to appear in Annales de l'IHP, Section Physique Théorique)

[2] Potential wells in high dimensions II, more about the one well case,

(to appear in Annales de l'IHP, Section Physique Théorique)

[Th] Colin J. Thompson

Mathematical statistical mechanics,

The Macmillan company New York (1972)

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