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Semiclassical expansions of the thermodynamic limit for a Schrödinger equation

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Semiclassical expansions of the thermodynamic limit for a Schrödinger equation
I. The one well case

by B.Helffer and J.Sjöstrand

§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) $K_m(h):=$

$$= \exp[-V^{(m)}(x)/2].\exp[h^2\Sigma_{k=1}^{m}\partial^2/\partial x_k^2].\exp[-V^{(m)}(x)/2]$$

with[1] :

(1.2) $V^{(m)}(x) = (1/4)\,\Sigma_{k=1}^{m} x_k^{\;2} - \Sigma_{k=1}^{m}\log ch(\sqrt{\nu/2}\;(x_k+x_{k+1}))$.

[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 :

$\mathrm{Lim}_{m\to\infty}(-\mathrm{Log}\ \mu_1(m;h,\nu)/m)$.

(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 :

$\mathrm{Lim}_{m\to\infty}(\mu_2(m;h,\nu)/\mu_1(m;h,\nu))$.

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 $[\mathrm{Ka}]_2$, 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 $[\mathrm{He-Sj}]_{1,4}$.

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

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

(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 :
$\mathrm{Lim}_{m\to\infty}\,(\lambda_1(m;h,\nu)/m)$.
(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 :
$\mathrm{Lim}_{m\to\infty}\,(\lambda_2(m;h,\nu) - \lambda_1(m;h,\nu))$.

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 $\mathrm{Lim}_{m\to\infty}\,(\lambda_1(m;h,\nu)/m)$
(2) asymptotic expansion of the limit as a formal series in h
(3) rapidity of the convergence as $m \to \infty$
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* $\Lambda(h,\nu) = \mathrm{Lim}_{m\to\infty} (\lambda_1(m;h,\nu)/m)$ *exists and admit 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 *s.t. for each j, there exists a constant* $C_j(\nu)$, *s.t.*

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

$C_j(\nu)$ *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) $[Sj]_{1,2}$.