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Exponential of a hamiltonian in large subsets of a lattice and applications

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after works with **L. AMOUR, C. CANCELIER, Ph. KERDELHUE,**

P. LEVY-BRUHL *and* **Ch. ROYER.**

1. Some models.

We are interested to quantum Hamiltonians for large systems of particles moving near the points of a large, but finite subset Λ of the lattice $\mathbb{Z}^d$. Near each point λ of Λ a particle, or a system of particles, moves in $\mathbb{R}^p$. The interaction between these particles is described by two functions:

- The interaction between particles moving near the same point λ of the lattice is described by a C^∞ real-valued, lower bounded function $A_\lambda(x)$ on $\mathbb{R}^p$. We assume that all derivatives of order ≥ 1 of this function are bounded, independently of λ.

- The interaction between particles moving near different points λ and μ of the lattice is described by a C^∞ real-valued function $B_{\lambda,\mu}(x, x')$ on $\mathbb{R}^{2p}$, which is bounded, like all its derivatives. A more precise hypothesis will be made in section 2.

Then, for each finite subset Λ of $\mathbb{Z}^d$, the potential V_Λ (function in $(\mathbb{R}^p)^\Lambda$) is defined by

$$V_\Lambda(x) = \sum_{\lambda\in\Lambda} A_\lambda(x_\lambda) + \sum_{(\lambda,\mu)\in\Lambda^2,\lambda\neq\mu} B_{\lambda,\mu}(x_\lambda, x_\mu) \tag{1.1}$$

where, for each point λ of Λ, x_λ denotes the corresponding set of variables. The hamiltonian is given by

$$H_\Lambda = -\frac{h^2}{2}\sum_{\lambda\in\Lambda} \Delta_{x_\lambda} + V_\Lambda(x). \tag{1.2}$$

In quantum statistical mechanics, the exponential $\exp(-\beta H_\Lambda)$, $(\beta > 0)$, plays an important role. A first description of the heat kernel of H_Λ, with estimations independent of the finite set Λ, was given in Sjöstrand [23]. More precisely, this article described an approximation, up to $\mathcal{O}(h^\infty)$, of this heat kernel, and introduced the notion of *0-standard function with exponential weight*. Later, the preprint [3] with L. Amour, C. Cancelier and P. Lévy-Bruhl described the heat kernel itself, using implicitely the concept of 0-standard function in a simple particular case (see also [4]). We prove, under suitable hypotheses, that the operator $\exp(-\beta H_\Lambda)$ has an integral kernel

$$U_\Lambda(x, y, \beta, h) = U_\Lambda^{(0)}(x, y, \beta, h) e^{-\psi_\Lambda(x,y,\beta,h)} \tag{1.3}$$

where $U_\Lambda^{(0)}$ is the heat kernel for the free Hamiltonian (without potential), and for ψ_λ we give estimates, (stated more precisely in section 2), meaning that this family of functions is in a particular case of $0-$standard functions.

There is a large literature of classical statistical mechanics for spin systems, with potentials V_Λ of the form (1.1). More generally, (see for example B. Simon [22]), it is common to associate, to each finite subset Q of $\mathbb{Z}^d$, (not only to sets of one or two points), a term A_Q which is a function on $(\mathbb{R}^p)^Q$, and then the potential V_Λ can be defined, instead of (1.1), (with obvious notations), by

$$V_\Lambda(x) = \sum_{Q \subseteq \Lambda} A_Q(x_Q). \tag{1.4}$$

Of course, an estimation of $\|A_Q\|_\infty$ as the diameter of Q increases is needed. It is possible, also, to take the sum on all finite subsets with a non void intersection with Λ, considering the variables x_λ, for points λ which are not in Λ, as given parameters. We shall see that, even when the potential V_Λ is of the particular form (1.1), the function ψ_Λ appearing in (1.3), at least when it is restricted in the diagonal, has a decomposition of the form (1.4), where the sum is taken on all the boxes Q contained in Λ, if Λ itself is a box. Moreover, the term corresponding to any box Q satisfies estimations involving the diameter of Q (See Proposition 2.2).

Then, once the decomposition of ψ_Λ, analogous to (1.4) is obtained, we can apply (or modify) the usual techniques of classical statistical mechanics for spin systems to prove, for the Schrödinger operator, results which are well known in classical statistical mechanics for spin systems. The first one is the *decay of "quantum correlations"*. See Theorem 3.1 for a precise statement, at least in a particular case. Similar rate results in classical statistical mechanics are well known: see section 3. Then, we can give other applications by a combination of the previous results and of usual techniques: rate of convergence of the mean value of observables for finite sets to their thermodynamic limit, mixing property of this thermodynamic limit, proof that this thermodynamic limit depends continuously of β in the domain of validity of our estimations (in other words, absence of phase transitions). See section 3, and the preprint [3].

In order to study other Hamiltonians than the Schrödinger operator, an attempt was made, with L. Amour and Ph. Kerdelhué [5], and with Ch. Royer [18], to study, not the heat kernel, but the pseudo-differential symbol of the operator $\exp(-\beta H_\Lambda)$, also with estimations independent of Λ. Unfortunately, we could apply our techniques only to operators of order 1, for example to the relativistic Hamiltonian

$$H_\Lambda = \sum_{\lambda \in \Lambda} \sqrt{1 - h^2 \Delta_{x_\lambda}} + V_\Lambda(x). \tag{1.5}$$

Our initial aim was to study the quantum Heisenberg model, with both large dimension and large spin. This would lead to Hamiltonians of second order on the manifold $(SU(2))^\Lambda$ of a similar form, but our techniques cannot be applied for this problem (brought to our attention by B. Helffer). See section 4.

2. Heat kernel of the Schrödinger equation.

We assume that, for each finite set Λ of $\mathbb{Z}^d$, V_Λ has the form (1.1), that the functions A_λ have all their derivatives of order ≥ 1 bounded independently of λ. We assume that there exists $\varepsilon \in]0, 1[$ such that $B_{\lambda,\mu}$ satisfies the following condition (H_ε).
(H_ε)
For each $m \geq 1$, there exists $C_m(\varepsilon) > 0$ such that $\sup_{\lambda \in \mathbb{Z}^d} \sum_{\mu \in \mathbb{Z}^d} \frac{\|B_{\lambda,\mu}\|_{C^m(\mathbb{R}^{2p})}}{\varepsilon^{|\lambda-\mu|}} \leq C_m(\varepsilon)$

If (H_ε) is satisfied, there exists $M_1(\varepsilon)$ and $M_2(\varepsilon)$, independent of Λ, such that:

$$\|\nabla_{x_\lambda} V_\Lambda\| \leq M_1(\varepsilon) \tag{2.1}$$

$$\sup_{\lambda \in \Lambda} \sum_{\mu \in \Lambda} \frac{\|\nabla_{x_\lambda} \nabla_{x_\mu} V_\Lambda\|}{\varepsilon^{|\lambda-\mu|}} \leq M_2(\varepsilon) \tag{2.2}$$

Theorem 2.1. *Under the previous hypotheses, the integral kernel $U_\Lambda(x, y, \beta, h)$ of $e^{-\beta H_\Lambda}$ can be written in the form*

$$U_\Lambda(x, y, \beta, h) \;=\; (2\pi\beta h^2)^{-p|\Lambda|/2}\; e^{-\frac{|x-y|^2}{2\beta h^2}}\; e^{-\psi_\Lambda(x,y,\beta,h)}, \tag{2.3}$$

where ψ_Λ is a C^∞ function in $(\mathbb{R}^p)^\Lambda \times (\mathbb{R}^p)^\Lambda \times [0, +\infty[$, depending on the parameter $h > 0$. Moreover, if (H_ε) is satisfied, for each finite subset Λ of $\mathbb{Z}^d$, we have, for all $\beta > 0$

$$\sup_{\lambda \in \Lambda} \|\nabla_\lambda \psi_\Lambda(.,.,\beta, h)\| \leq \beta M_1(\varepsilon) \tag{2.4}$$

and if $m \geq 2$, we have, for all points $\lambda^{(1)}, ..., \lambda^{(m-1)}$ in Λ,

$$\sum_{\mu \in \Lambda} \frac{\|\nabla_{\lambda^{(1)}} ... \nabla_{\lambda^{(m-1)}} \nabla_\mu \psi_\Lambda(.,.,\beta, h)\|_{L^\infty}}{\varepsilon^{\operatorname{diam}(\{\lambda_1,...\lambda_{m-1},\mu\})}} \leq \beta K_m(\varepsilon) \qquad \text{if} \qquad h\beta \leq M_2(\varepsilon)^{-1/2}. \tag{2.5}$$

where $K_m(\varepsilon)$ is independent of Λ.

The function ψ_Λ of Theorem 1.1 is obtained as the solution of the Cauchy problem (we wrote t instead of β)

$$\frac{\partial \psi_\Lambda}{\partial t} \;+\; \frac{x - y}{t} \;.\; \nabla_x \psi_\Lambda - \frac{h^2}{2} \Delta_x \psi_\Lambda \;=\; V_{\Lambda,\varepsilon}(x) \;-\; \frac{h^2}{2} |\nabla_x \psi_\Lambda|^2 \tag{2.6}$$

$$\psi_\Lambda(x,y,0,h,\varepsilon)=0 \tag{2.7}$$

First, a theorem of global existence, for a fixed Λ, is obtained, using a fixed point theorem, and a variant of the principle of maximum (see L. Amour and M. Ben-Artzi [2] for similar techniques, without the singular coefficient $\frac{x-y}{t}$). The variant of the principle of maximum is used again in the proof of (2.4) and (2.5). There is a relation between the inequality (2.5) and the notion of $0-$standard function of exponential type of [23].

The next step is a decomposition of ψ_Λ, similar to (1.4), in order to adapt the techniques of classical statistical mechanics. This will be obtained when Λ is a box of $\mathbb{Z}^d$, i.e. a set of the following form, where a_j and b_j are in $\mathbb{Z}$ and $a_j \leq b_j$ ($1\leq j\leq d$):

$$\Lambda=\{\lambda\in\mathbb{Z}^d, \quad a_j\leq\lambda_j\leq b_j \quad 1\leq j\leq d\} \tag{2.8}$$

Proposition 2.2. *If Λ is a box of $\mathbb{Z}^d$, the function $\psi_\Lambda(x,y,\beta,h)$ of Theorem 2.1 satisfies, if (H_ε) is satisfied and $h\beta\leq M_2(\varepsilon)^{-1/2}$,*

$$\psi_\Lambda(x,y,\beta,h)-\psi_\Lambda(0,y-x,\beta,h)=\sum_{Q\subseteq\Lambda}(T_Q\psi_\Lambda)(x,y,\beta,h) \tag{2.9}$$

where the sum is taken over all boxes contained in Λ, and $T_Q\psi_\Lambda$ is a function depending only on $x-y,\beta,h$ and on the variables x_λ and y_λ such that $\lambda\in Q$. For each integer $m\geq 1$, there exists $K_m(\varepsilon)$ such that, for each points $\lambda^{(1)}$, ..., $\lambda^{(m)}$ of Λ,

$$\|\nabla_{\lambda^{(1)}}...\nabla_{\lambda^{(m)}}(T_Q\psi_\Lambda)(.,.,\beta)\|\leq K_m(\varepsilon)\beta\varepsilon^{\mathrm{diam}(Q)} \qquad \text{if} \qquad h\beta\leq M_2(\varepsilon)^{-1/2}. \tag{2.10}$$

If $m=0$, this result is also valid for boxes Q non reduced to single points.

In particular, when it is restricted to the diagonal, $T_Q\psi_\Lambda$ depends only on the variables x_λ and y_λ such that $\lambda\in Q$, and we have a decomposition of ψ_Λ which is very similar to the form (1.4) usually supposed for the potential V_Λ in the literature of classical statistical mechanics. Theorem 1.1 and, again, the principle of maximum, are used in the proof of (2.10).

3. Applications: decay of quantum correlations, mixing property of states, etc.

In classical statistical mechanics, for each finite set Λ and for each $\beta>0$, the mean value of a bounded function f on $(\mathbb{R}^p)^\Lambda)$ by

$$E_{\Lambda,\beta}(f)=\frac{\int_{(\mathbb{R}^p)^\Lambda}e^{-\beta V_\Lambda(x)}f(x)dx}{\int_{(\mathbb{R}^p)^\Lambda}e^{-\beta V_\Lambda(x)}dx}. \tag{3.1}$$

Then, the correlation between two such functions f_1 and f_2 is defined by $\mathrm{cov}_{\Lambda,\beta}(f_1,f_2)=E_{\Lambda,\beta}(f_1f_2)-E_{\Lambda,\beta}(f_1)\ E_{\Lambda,\beta}(f_2)$. If f_j is a bounded function in $(\mathbb{R}^p)^{E_j})$ ($j=1,2$), where E_1 and E_2 are disjoint finite sets, we can define $\mathrm{cov}\Lambda, \beta(f_1, f_2)$ for each Λ containing E_1 and E_2. A classical problem is the estimation of the decay of this correlation with bounds which are independent of Λ, but depend on the distance between E_1 and E_2. For β small enough, see L. Gross [10], where a decomposition of the form (1.4) for the potential V_Λ is supposed. For β large enough, stronger hypotheses are needed: see Helffer-Sjöstrand [15], Sjöstrand [24], where the correlation is related with an eigenvalue of the Witten Laplacian of V_Λ acting on $1-$forms, Sjöstrand [25], and Bach-Möller [7].

A first application of the results of section 2 is the study, when β is small enough, of a quantum analogue of the correlation. Instead of functions, we consider, for each finite set Λ, bounded operators on the Hilbert space $\mathcal{H}_\Lambda = L^2((\mathbb{R}^p)^\Lambda)$. First, if A is such an operator, (a *local observable*), we can define the 'mean value' of A as

$$E_{\Lambda,\beta}(A) = \frac{tr\ \left(e^{-\beta H_\Lambda} A\right)}{tr\ \left(e^{-\beta H_\Lambda}\right)}\ . \tag{3.2}$$

If E_1 and E_2 are disjoints subsets of Λ, and if A_j is an operator in $\mathcal{H}_{E_j}$ ($j = 1, 2$)), we can define their quantum correlation by $\mathrm{cov}_{\Lambda,\beta}(A_1, A_2) = E_{\Lambda,\beta}(A_1A_2) - E_{\Lambda,\beta}(A_1)\ E_{\Lambda,\beta}(A_2)$, where the mean value is now (3.2).

We denote by $\mathrm{dist}(E, F)$ the distance, for the ℓ^∞ norm, of two subsets E and F of $\mathbb{Z}^d$. In the definitions of the mean value and of the correlation, we shall write $E_{\Lambda,\beta}(f)$ and $cov_{\Lambda,\beta}(f, g)$ instead of $E_{\Lambda,\beta}(A)$ and $cov_{\Lambda,\beta}(A, B)$ when A and B are multiplications by bounded functions f and g.

Theorem 3.1. *We assume that, for $|x_\lambda|$ large enough, $A_\lambda(x_\lambda) \geq c|x_\lambda|$, and that (H_ε) is satisfied ($0 < \varepsilon < 1$). Then, for each δ such that $\varepsilon < \delta < 1$, there exist $K(\varepsilon, \delta) > 0$ and $\beta_0(\varepsilon, \delta) > 0$ with the following properties. If E_1 and E_2 are disjoint sets of $\mathbb{Z}^d$, if f_j is a continuous, bounded functions on $(\mathbb{R}^p)^{E_j}$, ($j = 1, 2$), then we have, for each set Λ containing E_1 and E_2, for all h and β satisfying $h\beta \leq M_2(\varepsilon)^{-1/2}$, and $\beta \leq \beta_0(\varepsilon, \delta)$, for each box Λ containing E_1 and E_2,*

$$|cov_{\Lambda,\beta}(f_1, f_2)| \leq \inf\Big(\sharp(E_1), \sharp(E_2)\Big)\ \ \beta\ K(\varepsilon, \delta)\ \ \delta^{\mathrm{dist}(E_1,E_2)}\ \ \|f_1\|_\infty \|f_2\|_\infty. \tag{3.3}$$

When the operators A_1 and A_2 are no more multiplications, see the preprint [3] for a more precise statement. The preprint [3] gives more complicated statements, with stronger hypotheses, for Theorems 2.1, 2.2 and 3.1. The improvement of these results is a work in progress.

This estimation for the correlation of two local observables may be applied, to prove that, if $A \in \mathcal{L}(\mathcal{H}_Q)$ (Q fixed finite subset of $\mathbb{Z}^d$) is a local observable, and if $\beta > 0$, the following thermodynamic limit exists

$$\omega_\beta(A) = \lim_{n\to+\infty} E_{\Lambda_n,\beta}(A) \qquad \Lambda_n = \{-n, \ldots, n\}^d,$$

and to estimate the rate of convergence. Thus, this limit define a state on the $C^\star-$algebra associated to the lattice, and the decay of correlations is again applied to prove the mixing property, or the absence of phase transitions. See [3]. This kind of results is also obtained, with other hypotheses, by probabilistic methods: see [1], [8], [16], [17].

4. Pseudo-differential techniques: relativistic Hamiltonians.

It may be interesting to present earlier results where, instead of the integral kernel, the pseudo-differential symbol is studied. For each finite subset Λ of $\mathbb{Z}^d$, we consider an holomorphic function $f_\Lambda(x,\xi)$ on the following domain

$$\Omega_\Lambda(a) = \{(x,\xi) \in ((\mathbf{C}^p)^\Lambda \times (\mathbf{C}^p)^\Lambda, \qquad |\mathrm{Im}(x,\xi)|_\infty < a\} \tag{4.1}$$

where a is a positive constant, independent of Λ. We suppose also that, for some $M > 0$, also independent of Λ, such that

$$|\nabla_{x_\lambda} f_\Lambda(x,\xi)| + |\nabla_{\xi_\lambda} f_\Lambda(x,\xi)| \ \leq \ M \qquad \forall \lambda \in \Lambda, \qquad \forall (x,\xi) \in \Omega_\Lambda(a). \tag{4.2}$$

We assume also that $f_\Lambda(x,\xi$ is real when (x,ξ) is real, and lower bounded, with a lower bound which may depend on Λ. We shall say that a family (f_Λ) is in $S(a)$ if these conditions are satisfied. Then we associate to the symbol f the $h-$pseudo-differential operator $Op_h(f_\Lambda)$ defined formally by

$$(Op_h(f_\Lambda)u)(x) \ = \ (2\pi h)^{-n} \int_{(\mathbb{R}^p)^\Lambda \times (\mathbb{R}^p)^\Lambda} e^{\frac{i}{h}(x-y).\xi} f_\Lambda(\frac{x+y}{2}, \xi) u(y) \ dyd\xi \ .$$

where $n = p|\Lambda|$. With these hypotheses, $e^{-tOp_h(f_\Lambda)}$ is well defined, and we know, by the functional calculus of Helffer-Robert, that it is also a pseudo-differential operator, for each fixed Λ. The next theorem gives bounds which are uniform with respect to Λ (see [5] and [18] for the proof).

Theorem 4.1. *With the previous hypotheses, for each $b \in]0,a[$ and for each integer $m \geq 1$, there exists a constant $\varepsilon_m > 0$ and a family $(g_{\Lambda,h})$ in $S(b)$ such that*

$$e^{-tOp_h(f_\Lambda)} = Op_h(e^{-g_{\Lambda,h}}) \qquad \text{if} \qquad h^m|\Lambda| \leq \varepsilon_m \qquad 0 < t \leq 1. \tag{4.3}$$

The bounds of the derivatives of $g_{\Lambda,h}$, like in (4.2), are independent of h and Λ satisfying the condition of (4.3) (for m fixed). Moreover, $g_{\Lambda,h}$ has an asymptotic expansion in powers of h:

$$g_{\Lambda,h} = \sum_{j=0}^{m-1} E_\Lambda^{(j)}(x,\xi,t)h^j + h^m R_\Lambda^{(m)}(x,\xi,t,h) \tag{4.4}$$

where the families $E_\Lambda^{(j)}$ are in $S(b)$, $E_\Lambda^{(0)}(x,\xi,t) = tf_\Lambda(x,\xi)$ and, if (x,ξ) is in $\Omega_\Lambda(b)$ and is the previous conditions are satisfied, $|R_\Lambda^{(m)}(x,\xi,t,h)| \leq C_m|\Lambda|$, for some $C_m > 0$ independent of Λ.

The applications of Theorem 4.1 are limited due to the two restrictions: the order of the operator cannot be greater than 1, and the inequality between the Plank's constant and the number of elements of Λ makes impossible to apply it to the existence of a thermodynamic limit. With Ch. Royer, we considered for example the Hamiltonian (1.5) where $d = 1$, $\Lambda = \Lambda_n = \{-n, n\}$, where $n \to +\infty$, where the functions A_λ and $B_{\lambda,\mu}$ are holomorphic if $|\mathrm{Im} x|_\infty < 1$, real when x is real. Moreover $B_{\lambda,\mu}$ is uniformly bounded, and $B_{\lambda,\mu} = 0$ if $|\lambda - \mu| \neq 1$ (nearest neighbor interaction), while A_λ has it derivative of first order uniformly bounded, and, in the real domain, increases at infinity enough to give a sense to the following trace:

$$Z_{\Lambda_n}(t,h) = \frac{1}{|\Lambda_n|} \ln \left[(2\pi h)^{p|\Lambda_n|} \mathrm{Tr} \left(e^{-tH_{\Lambda_n}} \right) \right] \tag{4.5}$$

where H_{Λ_n} is now the relativistic Hamiltonian (1.5). Then the existence of the pressure $Z(t,h)$, limit of $Z_{\Lambda_n}(t,h)$ when $n \to +\infty$, is classical. See for example, Ruelle [21], where the rate of convergence $\mathcal{O}(n^{-1})$ is proved. Theorem 4.1 can be applied to prove that the pressure $Z(t,h)$ has an asymptotic expansion in powers of h. For this application, the relation between $|\Lambda|$ and h is not a difficulty. In particular, the inversion of the two limits ($n \to +\infty$ and $h \to 0$) is justified. This problem was brought to our attention (for another model) by B. Helffer.

The proof of Theorem 4.1, given with Ch. Royer in [18] relies on a still earlier result, with L. Amour and Ph. Kerdelhué [5], on the pseudo-differential calculus with large dimension. In particular, in [5] we give an estimation for the composed $f \star_h g$ of two symbols which are holomorphic and bounded in $\Omega_\Lambda(a)$ (i.e. the symbol such that $Op_h(f \star_h g) = Op_h(f) \circ Op_h(g)$. By Lemma 5.1 of [5] (see also Theorem 3.2 of [18]), this function is holomorphic and bounded in $\Omega_\Lambda(b)$ for $b \in]0, a[$ and, if we set $\|f\|_a = \sup_{(x,\xi)\in\Omega_\Lambda(a)} |f(x,\xi)|$, we have:

$$\|f \star_h g\|_b \leq \|f\|_a \; \|g\|_a \; \left(1 \; + \; \frac{\sqrt{2h}}{(a-b)\sqrt{\pi}} e^{-\frac{(a-b)^2}{h}} \right)^{4n} \qquad n = p|\Lambda|.$$

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