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Partial Differential Equations

States of a one dimensional quantum crystal

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Abstract

We construct states on a $C^\star$-algebra associated to a one dimensional lattice crystal. We also compute the mean value of an observable, not necessarily bounded, such as the dilation coefficient. This implies on one hand, a careful analysis of the heat kernel of the Hamiltonian associated to the crystal and, on the other hand, the study of the quantum correlations of two observables associated to two clusters of particules. ***To cite this article: L. Amour et al., C. R. Acad. Sci. Paris, Ser. I 336 (2003).***

Résumé

États d'équilibre d'un cristal quantique unidimensionnel. Nous construisons des états d'équilibre sur une $C^\star$ algèbre associée à un cristal quantique unidimensionnel. Nous étudions la valeur moyenne d'une observable, non nécessairement bornée, telle que le coefficient de dilatation. Ceci demande, d'une part, une analyse précise du noyau de la chaleur associé au cristal et, d'autre part, l'étude des corrélations quantiques de deux observables associés a deux amas de particules. ***Pour citer cet article : L. Amour et al., C. R. Acad. Sci. Paris, Ser. I 336 (2003).***

1. Introduction

Let us consider a quantum one dimensional lattice of particles, each of them moving in $\mathbb{R}^p$. For each finite subset Λ of $\mathbb{Z}$, we denote by $H_\Lambda(\varepsilon)$ the following differential operator in $(\mathbb{R}^p)^\Lambda$, depending on the Planck's constant h and on another small parameter ε (measuring the decay of interactions between particles of the lattice):

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

where $x=(x_\lambda)_{\lambda\in\Lambda}$ denotes the variable of $(\mathbb{R}^p)^\Lambda$, each variable x_λ being in $\mathbb{R}^p$. We suppose that the potential $V_{\Lambda,\varepsilon}\in C^\infty((\mathbb{R}^p)^\Lambda)$ is of the following form

$$V_{\Lambda,\varepsilon}(x) = \sum_{\lambda\in\Lambda} A(x_\lambda) + \sum_{\substack{\lambda,\mu\in\Lambda\\ \lambda\neq\mu}} \varepsilon^{|\lambda-\mu|} B_{\lambda-\mu}(x_\lambda, x_\mu), \quad x=(x_\lambda)_{(\lambda\in\Lambda)},$$

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where $A \in C^\infty(\mathbb{R}^p)$ and $B_\lambda \in C^\infty(\mathbb{R}^{2p})$ with the following hypotheses. We assume that $A(x) \sim C|x|$ at infinity (where $C > 0$), that all the B_λ are uniformly bounded, and that, for each integer $q \geqslant 1$, the derivatives of order q of A and B_λ are uniformly bounded.

For each $n \geqslant 1$, let $\Lambda_n = \{-n, \ldots, n\}$. We often write Λ instead of Λ_n. Let us remark that, the operator $\mathrm{e}^{-tH_{\Lambda_n}(\varepsilon)}$ appears explicitly in Theorems 2.1, 2.2, 3.1, 4.1 below. Therefore, a neat inspection of this operator is necessary. In [3], and actually for a d-dimensional $\Lambda_n = \{-n, \ldots, n\}^d$, we describe very carefully the integral kernel $U_\Lambda(x, y, t, h, \varepsilon)$ of $\mathrm{e}^{-tH_\Lambda(h)}$ (Sjöstrand began this study in [16]). Writing,

$$U_\Lambda(x, y, t, h, \varepsilon) = \left(2\pi t h^2\right)^{-p|\Lambda|/2} \mathrm{e}^{-|x-y|^2/(2th^2)} \mathrm{e}^{-\psi_\Lambda(x,y,t,h,\varepsilon)},$$

[3] contains sharp estimates on various derivatives of functions related to ψ with respect to x, y, t. For that, we shall find ψ as the solution of the Cauchy problem in $(\mathbb{R}^p)^\Lambda$

$$\frac{\partial \psi_\Lambda}{\partial t} + \frac{x-y}{t} \nabla_x \psi_\Lambda - \frac{h^2}{2} \Delta \psi_\Lambda = V_{\Lambda,\varepsilon}(x) - \frac{h^2}{2} |\nabla \psi_\Lambda|^2, \qquad \psi_\Lambda(x, y, 0, h, \varepsilon) = 0.$$

We prove first the global existence of ψ_Λ. Then, using a suitable variant of the maximum principle, we give estimations (not modulo $\mathcal{O}(h^\infty)$), in which the constants are independent on Λ. Some of these estimates are very much related to the concept of 0-standard functions, introduced by Sjöstrand [16], some other ones are newer.

Furthermore, ψ is decomposed as a sum of terms associated to clusters (cubes) of Λ, with an estimation of each term. These results are applied to the proof of Theorem 4.1.

2. States on a $C^\star$ algebra. Dilation coefficients

To each finite set Λ of $\mathbb{Z}$, we associate the Hilbert space $\mathcal{H}_\Lambda = L^2((\mathbb{R}^p)^\Lambda)$. If $\Lambda_1 \subseteq \Lambda_2$, we have a natural identification of $\mathcal{L}(\mathcal{H}_{\Lambda_1})$ into $\mathcal{L}(\mathcal{H}_{\Lambda_2})$. Classically, taking the closure of the union of all these $\mathcal{L}(\mathcal{H}_\Lambda)$, we can associate to our lattice a $C^\star$-algebra, denoted by $\mathcal{A}$ (cf. for example, Simon [15], end of Section II.1).

Theorem 2.1. *Let Q_0 be a finite subset of $\mathbb{Z}$, and let A be an element of $\mathcal{L}(\mathcal{H}_{Q_0})$ (a local observable). (Thus, for n large enough, Λ_n contains Q_0, and A can be considered as an element of $\mathcal{L}(\mathcal{H}_{\Lambda_n})$.) Then, with our hypotheses on the potentials, the following limit exists, if ε and ht are small enough (say $\varepsilon < \varepsilon_0$ and $ht < \varepsilon_0$):*

$$\omega(A) = \lim_{n \to +\infty} \frac{\operatorname{Tr}(\mathrm{e}^{-tH_{\Lambda_n}(\varepsilon)} A)}{\operatorname{Tr} \mathrm{e}^{-tH_{\Lambda_n}(\varepsilon)}}. \tag{1}$$

Moreover, for each compact K of $]0, \infty[^2$ such that $ht < \varepsilon_0$ in K, there are constants $C > 0$ and $\alpha > 0$ such that

$$\left| \omega(A) - \frac{\operatorname{Tr}(\mathrm{e}^{-tH_{\Lambda_n}(\varepsilon)} A)}{\operatorname{Tr} \mathrm{e}^{-tH_{\Lambda_n}(\varepsilon)}} \right| \leqslant C(C\varepsilon)^{\alpha n}, \quad \varepsilon < \varepsilon_0, \ (h, t) \in K.$$

Let us remark that $|\omega(A)| \leqslant \|A\|$, and therefore that the linear form $A \to \omega(A)$, defined on the union of all the $\mathcal{L}(\mathcal{H}_Q)$, can be extended to a state on $\mathcal{A}$. (It satisfies $\omega(I) = 1$ and $\omega(A^\star A) \geqslant 0$.) Recently, Minlos et al. [12,13] proved in the d-dimensional case, the existence of Gibbs states on $\mathcal{A}$ by similar limits, but for potentials of a very different type, and by techniques of Feynmann integrals, Albeverio et al. [1,2] also constructed Gibbs space by probabilistic methods.

The meaning of limits like (1) is the definition of mean values of an observable in all the lattice at temperature $\frac{1}{t}$. Our technique can be extended to observables which are not necessarily bounded, and therefore do not belong to the $C^\star$-algebra. For sake of simplicity, we shall restrict ourselves to the case where A is the multiplication by a polynomially bounded function.

Theorem 2.2. *With the notations of Theorem 2.1, let $f \in C^\infty((\mathbb{R}^p)^{Q_0})$ be a polynomially bounded function, and A be the operator (in $\mathcal{S}((\mathbb{R}^p)^{Q_0})$) of multiplication by f. (Then, if Λ contains Q_0, the operator $\mathrm{e}^{-tH_\Lambda(\varepsilon)} A$ is well defined in $\mathcal{L}(\mathcal{H}_\Lambda)$, and of trace class.) Then, if ht and ε are small enough, the limit (1) exists.*

For example, if $Q_0 = \{1, 2\}$, and if A is the multiplication by the function $f(x_1, x_2) = x_2 - x_1$, we can think than $\omega(A)$ is related to the dilation coefficient of the crystal.

3. Quantum mean energy

With our hypotheses, Sjöstrand [16] proved that the following limit (free energy) exists

$$P(t,\varepsilon) = \lim_{n\to+\infty} \frac{1}{|\Lambda_n|} \ln\bigl(\mathrm{Tr}\bigl(\mathrm{e}^{-tH_{\Lambda_n}(\varepsilon)}\bigr)\bigr).$$

He proved also that $P(t,\varepsilon)$ has an expansion in powers of h when $h \to 0$, while $\varepsilon > 0$ is fixed (cf. also [5] for other models). In the literature on solid state physics (Kittel [11] or Ashcroft and Mermin [4]), it appears that the partial derivative of $P(t,h)$ with respect of t is supposed to exist and to represent the mean energy $U(1/t,h)$ of the crystal (per site) at the temperature $1/t$. Therefore it can be interesting to prove mathematically that this derivative exists and that

$$\frac{\partial P(t,\varepsilon)}{\partial t} = -\lim_{n\to+\infty} \frac{1}{|\Lambda_n|} \frac{\mathrm{Tr}(H_{\Lambda_n}(\varepsilon)\,\mathrm{e}^{-tH_{\Lambda_n}(\varepsilon)})}{\mathrm{Tr}\,\mathrm{e}^{-tH_{\Lambda_n}(\varepsilon)}}. \tag{2}$$

Another application of our techniques is the proof of the following

Theorem 3.1. *With the preceding hypotheses, for $\varepsilon > 0$ and $th > 0$ small enough, $P(t,\varepsilon)$ is derivable with respect to t, and the derivative is given by* (2).

Let us mention that we estimate the speed of convergence in the limit in the right-hand side of (2).

We also remark that, in the case of a quadratic potential, Theorem 3.1 follows from the explicit computations of Royer [14].

4. Quantum correlation of local observables

In this section we study the correlation of two observables associated to two clusters of particles which are far one from the other. Similar results are proved in Helffer [6–8] and [10], in Sjöstrand [17] in the case of classical mechanics, and with very different hypotheses on the potential, and by a different method. In addition, Theorems 4.1–4.3 are strongly implied in the proof of Theorems 2.1, 2.2, 3.1.

For each finite set Λ of $\mathbb{Z}$, and for each (bounded, or satisfying suitable hypotheses) A in $\mathcal{H}_\Lambda$, we can define the 'mean value' of A as

$$E_{\Lambda,\varepsilon}(A) = \frac{\mathrm{Tr}(\mathrm{e}^{-tH_\Lambda(\varepsilon)}A)}{\mathrm{Tr}(\mathrm{e}^{-tH_\Lambda(\varepsilon)})}.$$

If Q_1 and Q_2 are disjoint subsets of Λ, and if A (resp. B) is an operator in $\mathcal{H}_{Q_1}$ (resp. in $\mathcal{H}_{Q_2}$), we can consider A and B as commuting operators in $\mathcal{H}_\Lambda$, and define their quantum correlation as

$$\mathrm{cov}_{\Lambda,\varepsilon}(A,B) = E_{\Lambda,\varepsilon}(AB) - E_{\Lambda,\varepsilon}(A)E_{\Lambda,\varepsilon}(B).$$

Theorem 4.1. *With the previous notations, for each integer m, there exists $\varepsilon_m > 0$ and $\alpha > 0$, such that, for each compact $K \subset]0,\infty[^2$ such that $ht < \varepsilon_m$ on K, there exists $C_m > 0$ with the following properties.*

(i) *For each interval Λ in $\mathbb{Z}$, for each disjoint subintervals $Q_1 \subseteq \Lambda$ and $Q_2 \subseteq \Lambda$ such that $|Q_j| \leqslant m$ $(1 \leqslant j \leqslant 2)$, $A \in \mathcal{L}(\mathcal{H}_{Q_1})$, $B \in \mathcal{L}(\mathcal{H}_{Q_2})$ we have*

$$\bigl|\mathrm{cov}_{\Lambda,\varepsilon}(A,B)\bigr| \leqslant C_m (C_m\varepsilon)^{\alpha\,\mathrm{dist}(Q_1,Q_2)} \|A\|\|B\|, \quad \varepsilon < \varepsilon_m,\ (h,t) \in K. \tag{3}$$

(ii) *If B is the multiplication by a bounded C^∞ function g on $(\mathbb{R}^p)^{Q_2}$, we have the same inequality if $|Q_1| \leqslant m$, but without any restriction on the number of elements of Q_2.*

(iii) *If A and B are the multiplications by bounded C^∞ functions f on $(\mathbb{R}^p)^{Q_1}$ and g on $(\mathbb{R}^p)^{Q_2}$, we have the estimate* (3) (*with C_m replaced by C_1*), *without any condition on the number of elements of Q_1 and Q_2.*

Let us consider now the case of two operators of multiplication by polynomially bounded functions.

Theorem 4.2. *With the notations of Theorem* 4.1*, for each interval* Λ *in* $\mathbb{Z}$*, for each disjoint subintervals* Q_1 *and* Q_2 *such that* $|Q_1| \leqslant m$*, if* A *is the multiplication by a* C^∞ *function* f *on* $(\mathbb{R}^p)^{Q_1}$ *such that, for some constant* $N_m(f)$*, we have* $|f(x)| \leqslant N_m(f)(1+|x|)^m$*, if* B *is the multiplication by by a bounded* C^∞ *function* g *on* $(\mathbb{R}^p)^{Q_2}$*, then we have* $|\mathrm{cov}_{\Lambda,\varepsilon}(A,B)| \leqslant C_m (C_m \varepsilon)^{\alpha\,\mathrm{dist}(Q_1,Q_2)} N_m(f) \|g\|_\infty$.

With the notations of Theorem 2.1, it follows from Theorem 4.1 that the sequence $\omega_n(A) = \mathrm{Tr}(\mathrm{e}^{-tH_{\Lambda_n}(h)}A)/\mathrm{Tr}\,\mathrm{e}^{-tH_{\Lambda_n}(h)}$ satisfies, for some $C>0$ and $\alpha>0$, if ht and ε is small enough, the estimation $|\omega_{m+n}(A) - \omega_m(A)| \leqslant C(C\varepsilon)^{\alpha m}$. To see that, we write the difference $\omega_{m+n}(A) - \omega_m(A)$ as a sum of quantum correlations between A and bounded functions, and we use Theorem 4.1 to estimate each term. Theorem 2.2 follows similarly from Theorem 4.2.

As a consequence of these theorems, we see that the state ω defined by (1) satisfies, for each local observables $A \in \mathcal{L}(\mathcal{H}_{Q_1})$ and $B \in \mathcal{L}(\mathcal{H}_{Q_2})$ $|\omega(AB) - \omega(A)\omega(B)| \leqslant C_m (C_m\varepsilon)^{\alpha\,\mathrm{dist}(Q_1,Q_2)} \|A\|\|B\|$.

For Theorem 3.1, we prove, using the same technique, that the sequence

$$X_n = \frac{(\mathrm{Tr}(H_{\Lambda_n}(h)\mathrm{e}^{-tH_{\Lambda_n}(h)})}{(\mathrm{Tr}\,\mathrm{e}^{-tH_{\Lambda_n}(h)})}$$

satisfies, under similar conditions, $|X_{m+n} - X_m - X_n| \leqslant C$, and then it follows from a classical result (cf. [9]) that the sequence X_n/n has a limit ℓ, and that $|X_n/n - \ell| \leqslant C/n$.

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