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A generalization of the Iorio–O'Carroll theorem to the case of lattice Hamiltonians

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Abstract. It is shown that a wide class of lattice Hamiltonians in solid state physics describing the system of N three-dimensional weakly interacting quasiparticles is unitarily equivalent to the one of corresponding Hamiltonians of the system of non-interacting quasiparticles.

Let us consider the operator

$$H_0 = \sum_{i=1}^{N} \Delta_i \tag{1}$$

acting in $l_2(\mathbb{Z}^{3N})$, where $\mathbb{Z}^3$ is a three-dimensional cubic lattice and Δ_i is the generalized lattice Laplacian acting via

$$(\Delta_i\varphi)(r_1 \ldots r_N) = \sum_{\mathbb{Z}^3} J_i(r)\varphi(r_1 \ldots r_{i-1}(r_i + r)r_{i+1} \ldots r_N) \tag{2}$$

where $r_i \in \mathbb{Z}^3$, $i = 1 \ldots N$ and $J_i(r)$ are exponentially decreasing functions: $|J_i(r)| < C_1 \exp(-C_2|r|)$. C_1, C_2 here and henceforth are some positive constants. Then let

$$V = \sum_{i<j} V_{ij}(r_i - r_j) + \sum_{i<j<l} W_{ijl}(r_i - r_j, r_j - r_l) \tag{3}$$

where each of the functions $V_{ij} \in l_{m_1}(\mathbb{Z}^3) \cap l_{m_2}(\mathbb{Z}^3)$ for some fixed m_1, m_2 such that $1 < m_1 < \frac{3}{2} < m_2 < \infty$, and each of the functions $W_{ijl} \in l_{m_1'}(\mathbb{Z}^6) \cap l_{m_2'}(\mathbb{Z}^6)$, where $1 < m_1' < \frac{3}{2} < m_2' < \infty$, and their Fourier transforms V_{ij} and W_{ijl} are the smooth functions on the torus. Finally, let us introduce the operator

$$H(\lambda) = H_0 + \lambda V \tag{4}$$

specified by some $\lambda \in \mathbb{R}$.

After Fourier transformation the operator $H(\lambda)$ becomes the operator $\tilde{H}(\lambda)$ acting in $L_2(T^{3N})$, where T^3 is a three-dimensional torus. In this so-called momentum representation we have the following expressions:

$$\tilde{H}(\lambda) = \tilde{H}_0 + \lambda \tilde{V} \qquad \tilde{H}_0 = -\sum_{i=1}^{N} \tilde{\Delta}_i \qquad \tilde{V} = \sum_{i<j} \tilde{V}_{ij} + \sum_{i<j<l} \tilde{W}_{ijl} \tag{5}$$

$$(\tilde{\Delta}_i\psi)(k_1 \ldots k_N) = \varepsilon_i(k_i)\psi(k_1 \ldots k_N) \tag{6}$$

$$(\tilde{V}_{ij}\psi)(k_1 \ldots k_N) = \int_{T^6} \tilde{V}_{ij}(k_i - k_j - k'_i + k'_j)\delta(k_i + k_j - k'_i - k'_j) \times \psi(k_1 \ldots k_{i-1}k'_i k_{i+1} \ldots k_{j-1}k'_j k_{j+1} \ldots k_N)\,\mathrm{d}k'_i\,\mathrm{d}k'_j \tag{7}$$

$$\varepsilon_i(k) = \sum_{\mathbb{Z}^3} J_i(r)\exp(\mathrm{i}(k, r)) \tag{8}$$

$$(\tilde{W}_{ijl}\psi)(k_1 \ldots k_N) = \int_{T^9} \tilde{W}_{ijl}(k_i - k_j - k'_i + k'_j, k_j - k_l - k'_j + k'_l)\delta(k_i + k_j + k_l - k'_i - k'_j - k'_l) \times \psi(k_1 \ldots k_{i-1}k'_i k_{i+1} \ldots k_{j-1}k'_j k_{j+1} \ldots k_{l-1}k'_l k_{l+1} \ldots k_N)\,\mathrm{d}k'_i\,\mathrm{d}k'_j\,\mathrm{d}k'_l \tag{9}$$

$$\tilde{V}_{ij}(k) = \sum_{\mathbb{Z}^3} V_{ij}(r)\exp(\mathrm{i}(k, r)) \tag{10}$$

$$\tilde{W}_{ijl}(k_1, k_2) = \sum_{\mathbb{Z}^6} W_{ijl}\exp[\mathrm{i}((k_1, r_1) + (k_2, r_2))] \tag{11}$$

where $(.,.)$ is a scalar product, $k_i \in T^3$, $i = 1, \ldots, N$. One can see from (8) that $\varepsilon(k)$ is the analytic function in some complex neighbourhood of a torus.

Evidently, the operator $H(\lambda)$ is bounded and self-adjoint.

The most natural source of such operators is solid state theory [1]. The operator (1) is the Hamiltonian describing, in the coordinate representation, the system of N quasiparticles (magnons, phonons, electrons, etc.) on a crystal lattice. Δ_i is the transfer operator describing hopping of the ith quasi-particle from site to site. $V_{ij}(.)$ is the pair potential of interaction and $W_{ijl}(.,.)$ is the three-particle potential. In a number of such systems quasi-particles interact weakly, which means that the value of $|\lambda|$ is sufficiently small.

The analogy to the N-particle Schrödinger operator is evident, and the Iorio-O'Carroll theorem on the unitary equivalence of operators describing free and interacting dynamics of weakly coupled three-dimensional systems for such Schrödinger operators [2, 3]. Here we will obtain the analogous result for lattice Hamiltonians. This result is important in physical applications because the spectrum of the free Hamiltonian H_0 is well known from formulae (5), (6) and (8), and it is absolutely continuous.

Theorem. For all sufficiently small $|\lambda|$ and for the functions $\varepsilon_i(k)$ of general position the operator $H(\lambda)$ is unitarily equivalent to the operator H_0.

Proof. The scheme of the proof is the same as in the continuous case in [3]. It follows from Kato's smoothness theorem [3] that our theorem is valid if the following conditions hold:

(i) $$\sup_{z \notin \mathbb{R}} \| |V_{ij}|^{1/2}(H_0 - z)^{-1}|V_{ln}|^{1/2}\| < \infty$$

(ii) $$\sup_{z \notin \mathbb{R}} \| |W_{ijl}|^{1/2}(H_0 - z)^{-1}|W_{nst}|^{1/2}\| < \infty$$

(iii) $$\sup_{z \notin \mathbb{R}} \| |V_{ij}|^{1/2}(H_0 - z)^{-1}|W_{lns}|^{1/2}\| < \infty$$

for all i, j, l, n, s, t. Let us begin with case (i) and let $l = i$, $n = j$.

(*a*) Let

$$\left(v_{ij}(q)\delta(k_i+k_j-k_i'-k_j')\prod_{l\neq i,j}\delta(k_l-k_l')\right)$$

be the kernel of the operator $|V_{i|}|^{1/2}$ in the momentum representation, where $q=\frac{1}{2}(k_i-k_j-k_i'+k_j')$. Then the kernel of the operator $T\equiv|V_{ij}|^{1/2}(H_0-z)^{-1}|V_{ij}|^{1/2}$ has the form

$$T(k,k',z)=J(K,z',q,q')\delta(K-K')\prod_{l\neq i,j}\delta(k_l-k_l') \tag{12}$$

where $k\equiv\{k_1\ldots k_N\}$; $K=k_i+k_j$;

$$\begin{aligned} J(K,z',q,q') &= \int_{T^3} v_{ij}(q-x)(\varepsilon_K(x)-z')^{-1}v_{ij}(x-q')\,\mathrm{d}x \\ z' = z-\sum_{l\neq i,j}\varepsilon(k_l) &\qquad \varepsilon_K(x)=\varepsilon_i(K/2+x)+\varepsilon_j(K/2-x). \end{aligned} \tag{13}$$

The function $J(z')$ (we have omitted the variables K, q, q') can be represented in Gelfand-Lereh form [4]:

$$J(z')=\int_{-\infty}^{+\infty}\mathrm{d}\zeta(\zeta-z')^{-1}I(\zeta) \tag{14}$$

$$I(\zeta)=\int_{\varepsilon_K(x)=\zeta} v_{ij}(q-x)v_{ij}(x-q')\,\mathrm{d}w(\zeta) \tag{15}$$

where formally $\mathrm{d}w(\zeta)=\mathrm{d}w/\mathrm{d}\zeta$ ($\mathrm{d}w=\mathrm{d}s(x)|\nabla\varepsilon_K(x)|^{-1}$, $\mathrm{d}s(x)$ is the Euclidean element of the area of the surface given by $\varepsilon_K(x)=\zeta$).

Let us show that $I(\zeta)$ is a bounded function of the Hölder type [3]. It is true if the function $I'(\zeta)$ is also of the Hölder type, where

$$I'(\zeta)=\int_{\varepsilon_K(x)=\zeta} 1\,\mathrm{d}w(\zeta) \tag{16}$$

because a locally smooth function is equivalent to a constant.

Let us consider the function

$$\sigma(t)=\int_{-\infty}^{+\infty}\exp(\mathrm{i}t\zeta)I'(\zeta)\,\mathrm{d}\zeta. \tag{17}$$

It is easy to check that

$$\sigma(t)=\int_{T^3}\exp(\mathrm{i}t\varepsilon_K(x))\,\mathrm{d}x. \tag{18}$$

The asymptotics of the integral (18) appearing in a stable way in the general position are cited in [4]:

$$\sigma(t)=\begin{cases} Ct^{-3/2} \\ Ct^{-(1+0.5/\mu)} & \qquad 0<\mu\leqslant 7 \\ Ct^{-(1+1/\mu)} \end{cases}$$

and the corresponding singularities of the function $I'(\lambda)$, and respectively of $I(\lambda)$, are the following:

$$I(\lambda)=\begin{cases}\zeta^{1/2}\\ \zeta^{1/2\mu}\\ \zeta^{1/\mu}.\end{cases} \tag{19}$$

Consequently, the function $I(\lambda)$ is of the Hölder type, and its Hilbert transform is bounded. It is seen from (12) that the operator T can be decomposed by the direct integral decomposition [3]. Because of operator, its norm is uniformly bounded for all $z\notin\mathbb{R}$ (see [3]).

(*b*) Now let $l=j$, $n\neq i$ and $|V_{ij}|^{1/2}\equiv g_{ij}$. If $\mathrm{Im}(z)>0$ then

$$g_{ij}(H_0-z)^{-1}g_{jn}=-\mathrm{i}\int_0^\infty \mathrm{d}t\ \mathrm{e}^{\mathrm{i}tz}g_{ij}(\mathrm{e}^{-\mathrm{i}tH_0})g_{ij}$$

$$\|g_{ij}(r_i-r_j)\,\mathrm{e}^{-\mathrm{i}t(\Delta_i+\Delta_j)}g_{jn}(r_j-r_n)\varphi(r_1\ldots r_n)\|=\|g_{ij}(r_i-r_j)(\mathrm{e}^{-\mathrm{i}t\Delta_i})g_{jn}(r_j-r_n)\varphi'(r_1\ldots r_N)\|$$

where $\varphi'=(\mathrm{e}^{-\mathrm{i}t\Delta_i})\varphi$ and $\|\varphi'\|=\|\varphi\|$. Here we have used the unitarity of the operators $\mathrm{e}^{-\mathrm{i}\Delta_i}$, $i=1,\ldots,N$, and the fact that such an operator commutes wih the operator of multiplication by the function of the variables which do not contain r_i.

Let us now calculate the partial norm

$$\|g_{ij}(r_i-r_j)(\mathrm{e}^{-\mathrm{i}t\Delta_i})g_{jn}(r_j-r_n)\varphi'(r_1\ldots r_N)\|_{l_2(r_j)}.$$

Lemma. $\|\mathrm{e}^{-\mathrm{i}t\Delta_i}\|_{1,\infty}\leqslant(Ct)^{-3/2}$ (where $\|.\|_{1,\infty}\colon l_1(\mathbb{Z}^3)\to l_\infty(\mathbb{Z}^3)$).

Proof. The operator $\mathrm{e}^{-\mathrm{i}t\Delta_i}$ acts as a convolution with the function

$$G(r)=\int_{T^3}\exp(-\mathrm{i}t\varepsilon(k)+(r,k))\,\mathrm{d}k. \tag{20}$$

But $|G(r)|\leqslant(Ct)^{-3/2}$, because the second derivatives of the function $\varepsilon'(k)\equiv\varepsilon(k)-(k,r/t)$ coincide with those of the function $\varepsilon(k)$, so in general the function $\varepsilon(k)$ can possess Morse critical points only. After this the proof is evident. □

Evidently, $\varphi'(r_j)\in l_2(\mathbb{Z}^3)$; $V_{ij}(r_i-r_j)\in l_p(\mathbb{Z}^3)$ uniformly by r_i; $V_{jn}(r_j-r_n)\in l_p(\zeta^3)$ uniformly by r_n. It follows from Hölder inequalities that $g_{jn}\varphi'\in l_s(\mathbb{Z}^3)$, where $s=2p/(p+1)$, $\|g_{jn}\varphi'\|_{s,r_i}\leqslant\|V_{jn}\|^{1/2}\|\varphi'\|_{2,r_i}$. But from Riesz–Thorin interpolation theorem [5] one can conclude from the inequality $\|\mathrm{e}^{-\mathrm{i}t\Delta_i}\|_{1,\infty}\leqslant(Ct)^{-3/2}$ and from the equality $\|\mathrm{e}^{-\mathrm{i}t\Delta_i}\|_{2,2}=1$ that $\|\mathrm{e}^{-\mathrm{i}t\Delta_i}\|_{s,s'}\leqslant(Ct)^{(0.5-s^{-1})}$, where $s^{-1}+s'^{-1}=1$. Consequently, $\mathrm{e}^{-\mathrm{i}t\Delta_i}(g_{jn}\varphi')\in l_{s'}(\mathbb{Z}^3)$, and

$$\|\mathrm{e}^{-\mathrm{i}t\Delta_i}(g_{jn}\varphi')\|_{s'}\leqslant(Ct)^{-3/2p}\|V_{jn}\|_p^{1/2}\|\varphi'\|_2.$$

Again using the Hölder inequality one obtains

$$\|g_{ij}(\mathrm{e}^{-\mathrm{i}t\Delta_i})g_{jn}\varphi'\|_{2,r_i}\leqslant(Ct)^{-3/2}\|V_{ij}\|_p^{1/2}\|V_{jn}\|_p^{1/2}\|\varphi\|_{2,r_i}. \tag{21}$$

Integrating (21) by other variables one concludes that

$$\|g_{ij}(\mathrm{e}^{-\mathrm{i}t\Delta_i})g_{jn}\varphi'\|_2\leqslant(Ct)^{-3/2p}\|V_{ij}\|_p^{1/2}\|V_{jn}\|_p^{1/2}\|\varphi\|_2. \tag{22}$$

Remembering that $V_{ij}(r) \in l_p(\mathbb{Z}^3) \cap l_q(\mathbb{Z}^3)$ for all i, j and $1 < p < \frac{3}{2} < q < \infty$, one sees from (22) (assuming $\mathrm{Im}(z) > 0$) that

$$\|g_{ij}(H_0 - z)^{-1} g_{jn}\| \leqslant \int_0^\infty \mathrm{d}t \, \mathrm{e}^{-t(\mathrm{Im}(z))} \min_{s=p,q} [(Ct)^{-3/2s} \| V_{ij}\|_s^{1/2} \| V_{jn}\|_s^{1/2}] < \infty.$$

The proof of case (b) is completed.

(c) Now let $l \neq i, j$, $n \neq i, j$. The proof of this case is almost the same as that of case 3 in the proof of the Iorio-O'Carroll theorem in [3]. Without loss of generality let $i = 1$, $j = 2$, $l = 3$, $n = 4$. Then

$$\begin{aligned} |(\varphi, g_{12}(\mathrm{e}^{-\mathrm{i}tH_0}) g_{34}\psi)| & \\ &= |(\mathrm{e}^{\mathrm{i}t(\Delta_3+\Delta_4)}\varphi, g_{12}\, \mathrm{e}^{-\mathrm{i}t(H_0-\Delta_3-\Delta_4)} g_{34}\psi)| \\ &= |(g_{34}\, \mathrm{e}^{\mathrm{i}t(\Delta_3+\Delta_4)}\varphi, g_{12}\, \mathrm{e}^{-\mathrm{i}t(H_0-\Delta_3-\Delta_4)}\psi)| \\ &\leqslant \|g_{34}\, \mathrm{e}^{\mathrm{i}t(\Delta_3+\Delta_4)}\varphi\| \, \|g_{12}\, \mathrm{e}^{-\mathrm{i}t(\Delta_1+\Delta_2)}\psi\|. \end{aligned}$$

In the first step we have used the fact that g_{12} and $(\Delta_3 + \Delta_4)$ commute, in the second step that g_{34} commutes with $(H_0 - \Delta_3 - \Delta_4)$, and in the last step that g_{12} and $(H_0 - \Sigma_{i=1}^4 \Delta_i)$ commute.

It is known from the corollary to theorem 13.25 of [3] that the operator A is H-smooth if $\sup_{z \notin \mathbb{R}} \|A(H-z)^{-1}A^*\| < \infty$. So the operator g_{ij} is $(\Delta_i + \Delta_j)$ smooth. Thus,

$$\begin{aligned} \int_{-\infty}^{+\infty} & \|g_{34}\, \mathrm{e}^{\mathrm{i}t(\Delta_3+\Delta_4)}\varphi\| \, \|g_{12}\, \mathrm{e}^{-\mathrm{i}t(\Delta_1+\Delta_2)}\psi\| \, \mathrm{d}t \\ &\leqslant \left(\int_{-\infty}^{+\infty} \|g_{34}\, \mathrm{e}^{\mathrm{i}t(\Delta_3+\Delta_4)}\varphi\|^2 \, \mathrm{d}t \right)^{1/2} \left(\int_{-\infty}^{+\infty} \|g_{12}\, \mathrm{e}^{-\mathrm{i}t(\Delta_1+\Delta_2)}\psi\|^2 \, \mathrm{d}t \right)^{1/2} \\ &\leqslant \|g_{34}\|_{(\Delta_3+\Delta_4)} \|g_{12}\|_{(\Delta_1+\Delta_2)} \|\varphi\| \, \|\psi\| \end{aligned}$$

see the definition of the norm $\|\cdot\|_H$ in [3] from which it follows that

$$\int_{-\infty}^{+\infty} |(\varphi, g_{12}\, \mathrm{e}^{-\mathrm{i}tH_0} g_{34}\psi)| \, \mathrm{d}t \leqslant C \|\varphi\| \, \|\psi\|. \tag{23}$$

For $\mathrm{Im}(z) > 0$

$$(\varphi, g_{12}(H_0 - z)^{-1} g_{34}\psi) = -\mathrm{i} \int_0^\infty \mathrm{e}^{\mathrm{i}tz} (\varphi, g_{12}\, \mathrm{e}^{-\mathrm{i}tH_0} g_{34}\psi) \, \mathrm{d}t$$

and consequently

$$\sup_{z \notin \mathbb{R}} \| |V_{12}|^{1/2} (H_0 - z)^{-1} |V_{34}|^{1/2} \| < \infty \tag{24}$$

and the proof of case (i) is completed.

The proof of case (ii) when $i = n$, $j = s$, $l = t$, is the same as in (a) above. Instead of the function $\varepsilon_K(x)$ we should consider the function

$$\varepsilon_K(x_1, x_2) \equiv \varepsilon_i[\tfrac{1}{3}(K - 2x_1 - x_2)] + \varepsilon_j[\tfrac{1}{3}(K + x_1 - x_2)] + \varepsilon_l[\tfrac{1}{3}(K + x_1 + 2x_2)]$$

and all estimates are only improved. If $i = n$, $j = s$, $l \neq t$ then the proof is the same as in (a). If $i = n$, $j \neq s, t$, $l \neq s, t$ then the proof is the same as in (b). Finally, if $i \neq n, s, t$, $j \neq n, s, t$, $l \neq n, s, t$ then the proof is the same as in (c).

Analogously, for case (iii) the correspondences are as follows:

$$i = l, j = n: (a) \qquad i = l, j \neq n, s: (b) \qquad i \neq l, n, s, j \neq l, n, s: (c).$$

This completes the proof. □

Finally we will briefly discuss the obtained result.

(i) There can be no such theorem in one- and two-dimensional cases [1] as well as in the continuous case [3].

(ii) There are some important examples in solid state physics in which the degeneration of some critical points of the functions $\varepsilon_K(k_1 \ldots k_s) \equiv \Sigma_{i=1}^{s} \varepsilon(k_i) + \varepsilon(K - \Sigma_{i=1}^{s} k_i)$ are not of general position (see [1, 6]). Under this it was shown that the theorem is not valid.

(iii) It is interesting to note that, from the proof above, only when the interaction is pair-wise is the upper bound for the critical number of particles at which the theorem is valid $N_c \approx \lambda^{-1/2}$. However it is known (see [1]) that $N_c \approx \lambda^{-1}$. The weakness of this estimate is connected to the roughness of the norm estimate technique.

(iv) The extension of the theorem to dimensions higher than three and to cases of not only 2- and 3- but also 4-, ..., N-particle potentials is evident.

(v) The physically important corollary is that in three-dimensional systems of N weakly interacting quasiparticle bound states, resonances and singular spectra do not exist, and the Hamiltonian possesses wave operators which are complete.

(vi) It is easy to prove the theorem for the case when, for the first quasiparticle, $J_1(r) \equiv 0$. This means that this quasiparticle is motionless and we have the problem of an impurity on a crystal lattice weakly interacting with $N-1$ quasiparticles. Under this condition parts (a) and (c) of the proof remain unchanged but in part (b) one has to use the techniques of part (c).

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