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# THE EXISTENCE OF ENERY GAPS FOR THREE-DIMENSIONAL SYSTEMS WITHOUT LONG RANGE ORDER

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The problem of the existence of the forbidden gaps in the energy spectrum of electrons in systems without long range order is an old one [1,2]. While for completely disordered systems one cannot expect to have forbidden gaps, the general belief is that the existence of energy gaps depends to a great degree on the short range order and it is generally independent of the degree of long range order. For one-dimensional systems, this has been proved by Borland [3] but to our best knowledge no proof exists for higher dimensional systems. The aim of this letter is to provide such a proof. The surprising fact is that the proof is quite simple, almost trivial. In fact, after the completion of this work, we became aware of the fact that the basic ideas underlying the two steps of the proof were known* for a long time:
i) the "shift" of the disorder from the potential energy to the kinetic energy has been used long time ago by Gubanov [4];
ii) the control of the perturbation theory can be achieved by general theory of singular perturbations [5].

We shall write the proof for three-dimensional systems, but in fact, the proof does not depend on the dimension of the system.

Let $V(\vec{x})$ be a periodic function and

$$H_0 = -\frac{\hbar^2}{2m}\Delta_{\vec{x}} + V(\vec{x}) \equiv T + V \tag{1}$$

be the Hamiltonian representing the "ideal" periodic system. About V we shall suppose that

$$\lim_{a\to\infty} \left\| V\frac{1}{T+a}\right\| = 0 . \tag{2}$$

The condition (2) is usual in nonrelativistic quantum mechanics and is a rather weak one; in particular, it is enough that (in three-dimensions) $V(\vec{x})$ is square integrable on the unit cell (ref. [6] Th. XIII96).

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Let $g_i(\vec{x})$, $i=1,2,3$ be a $C^3$ vector function with the property that

$$\sup_{\vec{x}\in R^3} \max_{i,j=1,2,3} \left|\frac{\partial g_i}{\partial x_j}\right| \leq 1$$

$$\sup_{\vec{x}\in R^3} \max_{i,j,k=1,2,3} \left|\frac{\partial^2 g_i}{\partial x_j \partial x_k}\right| \leq 1 \qquad (3)$$

$$\sup_{\vec{x}\in R^3} \max_{i,j,k,\ell=1,2,3} \left|\frac{\partial^3 g_i}{\partial x_j \partial x_k \partial x_\ell}\right| \leq 1 .$$

We shall represent disorderd systems by the following type of Hamiltonians

$$H_\epsilon = -\frac{\hbar^2}{2m}\Delta_{\vec{x}} + V(\vec{x}+\epsilon\vec{g}(\vec{x})) = T + V_\epsilon , \qquad (4)$$

where $\epsilon$ is a positive number. The periodic system is recovered by $\epsilon = 0$. In general, for small $\epsilon$ there is still a short range order, but at long distances the order is lost, the characteristic length being of order $a/\epsilon$, where a is the linear dimension of the unit cell. Our result is:

Theorem 1. Suppose that $[a,b]\subset R$ is in the resolvent set of $H_0$, $[a,b]\subset \rho(H_0)$. Then for sufficiently small $\epsilon$, there exist $a\leq a_\epsilon < b_\epsilon \leq b$ such that $[a_\epsilon, b_\epsilon] \subset \rho(H_\epsilon)$. Moreover,

$$\lim_{\epsilon\to 0} a_\epsilon = a,$$

$$\lim_{\epsilon\to 0} b_\epsilon = b. \qquad (5)$$

Proof of Th.1. Before entering the technicalities, let us give the main ideas. The difficulty is due to the fact that the problem does not have a small parameter on which a perturbation approach should be based. Then, in the first step, we shall shift by a change of variable, the disorder from the potential energy to the kinetic energy. In the new representation, the kinetic energy can be written as the sum of the usual term $-\frac{\hbar^2}{2m}\Delta$ and a perturbation. The price is that altough the perturbation term contains $\epsilon$ as a factor, it is rather singular. The second step is to show that this singular perturbation can be controlled.

1st. step. There exists $\epsilon_0 > 0$ such that for $0 < \epsilon \leq \epsilon_0$

$$J_\epsilon(\vec{x}) = \det|\delta_{ij} + \epsilon \frac{\partial g_i(\vec{x})}{\partial x_j}| \geq \frac{1}{2} . \tag{6}$$

Then one can define the following unitary operator $U_\epsilon : L^2(\mathbf{R}^3) \to L^2(\mathbf{R}^3)$

$$(U_\epsilon f)(\vec{x}) = [J_\epsilon(\vec{x})]^{1/2} f(\vec{x} + \epsilon \vec{g}(\vec{x})) . \tag{7}$$

Consider

$$\tilde{H}_\epsilon = U_\epsilon^* H_\epsilon U_\epsilon = U_\epsilon^* T U_\epsilon + U_\epsilon^* V_\epsilon U_\epsilon . \tag{8}$$

By direct computation

$$\begin{aligned} &(U_\epsilon^* V_\epsilon U_\epsilon f)(\vec{x}) = V(\vec{x}) f(\vec{x}), \\ &U_\epsilon^* T U_\epsilon = T + \epsilon D_\epsilon , \end{aligned} \tag{9}$$

where $D_\epsilon$ has the following from

$$D_\epsilon = \frac{\hbar^2}{2m}[\sum_{i,j=1}^{3} A_{ij}(\vec{x}) \frac{\partial^2}{\partial x_i \partial x_j} + \sum_{j=1}^{3} B_j(\vec{x}) \frac{\partial}{\partial x_j} + C(\vec{x})] \tag{10}$$

and all coefficients appearing in (10) are uniformly bounded with respect to $\vec{x} \in \mathbf{R}^3$ and $\epsilon \in (0, \epsilon_0)$, by a constant K.

2nd. step. From the functional calculus, one has for $z \in R(d) = \{z \in \mathbf{C} \mid \mathrm{Re}\, z \leq -d < 0\}$

$$\begin{aligned} &\frac{\hbar^2}{2m} \left\| \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \frac{1}{T - z} \right\| \leq 1 , \\ &\frac{\hbar^2}{2m} \left\| \frac{\partial}{\partial x_i} \frac{1}{T - z} \right\| \leq \left(\frac{\hbar^2}{8md}\right)^{1/2} . \end{aligned} \tag{11}$$

From (10) and (11) it follows that for $0 < \epsilon < \epsilon_0$ and $z \in R(d)$

$$\left\| D_\epsilon \frac{1}{T - z} \right\| \leq k(d) . \tag{12}$$

The condition (2) assures the existence of $d_0 < \infty$ such that for $z \in R(d_0)$

$$\|V\frac{1}{T-z}\| \leq \frac{1}{2}. \qquad (13)$$

Then using the identity

$$\frac{1}{T+V-z} = \frac{1}{T-z}[1 + V\frac{1}{T-z}]^{-1} \qquad (14)$$

one obtains for $0 < \epsilon < \epsilon_0$, $z \in R(d_0)$

$$\|D_\epsilon \frac{1}{T+V-z}\| \leq 2k(d_0) \qquad (15)$$

and the use of Th.VI 5.12 from Kato's book [5] finishes the proof of the theorem.

Remark

Even without relying on the general theorems of perturbation theory, the proof of the Th.1 is immediate. Suppose $\epsilon < [2k(d_0)]^{-1}$. The following formula valid for $\mathrm{Re}\, z_0 < -d_0$

$$\frac{1}{T+V+\epsilon D_\epsilon - z} = \frac{1}{T+V-z}\{(1+\epsilon D_\epsilon \frac{1}{T+V-z_0}) \times$$

$$\times [1 + \epsilon(z_0 - z)(1+\epsilon D_\epsilon \frac{1}{T+V-z_0})^{-1} D_\epsilon \frac{1}{T+V-z_0} \cdot \frac{1}{T+V-z}]\}^{-1}$$

shows that $(T+V+\epsilon D_\epsilon - z)^{-1}$ exists for all $z \in \rho(T+V)$ satisfying

$$\|\epsilon(z-z_0)(1+\epsilon D_\epsilon \frac{1}{T+V-z_0})^{-1} D_\epsilon \frac{1}{T+V-z_0} \frac{1}{T+V-z}\| < 1. \qquad (16)$$

In particular, if $\lambda$ is middle of a gap of magnitude $\Delta E$ then $\lambda \in \rho(H_\epsilon)$ if

$$\epsilon < \frac{\Delta E(1 - 2\epsilon k(d_0))}{4k(d_0)(\lambda + d_0)} . \qquad (17)$$

Applied to concrete cases, the inequality (17) gives a (very rough) estimate of $\epsilon$, for which a forbidden gap still exists.

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