The existence of energy gaps for three-dimensional systems without long-range order

1981 J. Phys. A: Math. Gen. 14 L109

(http://iopscience.iop.org/0305-4470/14/5/001)

J. Phys. A: Math. Gen. 14 (1981) L109–L112. Printed in Great Britain

LETTER TO THE EDITOR

The existence of energy gaps for three-dimensional systems without long-range order

A Nenciu† and G Nenciu†

Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, SU-141980, Dubna, USSR

Received 6 January 1981

Abstract. The existence of energy gaps in the electronic spectrum for three-dimensional systems having short-range order but without long-range order, is proved.

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 (Lieb and Mattis 1966, Mott and Davis 1979). 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 (1961) 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 was used many years ago by Gubanov (1954, 1955);

(ii) the control of perturbation theory can be achieved by the general theory of singular perturbations (Kato 1966).

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

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

$$H_0 = -(\hbar^2/2m)\Delta_x + V(\boldsymbol{x}) \equiv T + V \qquad (1)$$

be the Hamiltonian representing the 'ideal' periodic system. Concerning V, we shall suppose that

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

Condition (2) is usual in nonrelativistic quantum mechanics and is a rather weak one; in particular, it is enough that (in three dimensions) $V(\boldsymbol{x})$ is square integrable on the unit cell (Reed and Simon 1978, Th. XIII 96).

† Permanent address: Central Institute of Physics, PO Box 5206, Bucharest, Romania

‡ We are grateful to Drs L Banyai and N Angelescu for pointing out to us the relevant literature.

0305-4470/81/050109+04$01.50

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

$$\begin{aligned}
&\sup_{\boldsymbol{x}\in\mathbb{R}^3} \max_{i,j=1,2,3} \left|\frac{\partial g_i}{\partial x_j}\right| \leqslant 1 \\
&\sup_{\boldsymbol{x}\in\mathbb{R}^3} \max_{i,j,k=1,2,3} \left|\frac{\partial^2 g_i}{\partial x_j\, \partial x_k}\right| \leqslant 1 \qquad (3)\\
&\sup_{\boldsymbol{x}\in\mathbb{R}^3} \max_{i,j,k,l=1,2,3} \left|\frac{\partial^3 g_i}{\partial x_j\, \partial x_k\, \partial x_l}\right| \leqslant 1.
\end{aligned}$$

We shall represent disordered systems by the following type of Hamiltonian

$$H_\varepsilon = -\hbar^2\Delta_x/2m + V(\boldsymbol{x}+\varepsilon\boldsymbol{g}(\boldsymbol{x})) \equiv T + V_\varepsilon \qquad (4)$$

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

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

$$\begin{aligned}
&\lim_{\varepsilon\to 0} a_\varepsilon = a \\
&\lim_{\varepsilon\to 0} b_\varepsilon = b.
\end{aligned} \qquad (5)$$

Proof of Theorem 1. Before mentioning 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 could be based. Then, in the first step, we shall shift the disorder, by a change of variable, 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 $-\hbar^2\Delta/2m$, and a perturbation. The price is that although the perturbation term contains ε as a factor, it is rather singular. The second step is to show that this singular perturbation can be controlled.

Step 1. There exists $\varepsilon_0>0$ such that for $0<\varepsilon\leqslant\varepsilon_0$

$$J_\varepsilon(\boldsymbol{x}) = \det|\delta_{ij} + \varepsilon\ \partial g_i(\boldsymbol{x})/\partial xj| \geqslant \tfrac{1}{2}. \qquad (6)$$

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

$$(U_\varepsilon f)(\boldsymbol{x}) = [J_\varepsilon(\boldsymbol{x})]^{1/2} f(\boldsymbol{x}+\varepsilon\boldsymbol{g}(\boldsymbol{x})). \qquad (7)$$

Consider

$$\tilde{H}_\varepsilon = U_\varepsilon H_\varepsilon U_\varepsilon^* = U_\varepsilon T U_\varepsilon^* + U_\varepsilon V_\varepsilon U_\varepsilon^*. \qquad (8)$$

By direct computation

$$\begin{aligned}
&(U_\varepsilon V_\varepsilon U_\varepsilon^* f)(\boldsymbol{x}) = V(\boldsymbol{x}) f(\boldsymbol{x}) \\
&U_\varepsilon T U_\varepsilon^* = T + \varepsilon D_\varepsilon
\end{aligned} \qquad (9)$$

where D_ε has the following form

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

and all coefficients appearing in (10) are uniformly bounded with respect to $\boldsymbol{x} \in \mathbb{R}^3$ and $\varepsilon \in (0, \varepsilon_0)$, by a constant K.

Step 2. From the functional calculus, one has for $z \in R_d = \{z \in \mathbb{C} \mid \mathrm{Re}\, z \leq -d < 0\}$

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

From (10) and (11) it follows that for $0 < \varepsilon < \varepsilon_0$ and $z \in R(d)$

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

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

$$\|V(T-z)^{-1}\| \leq \tfrac{1}{2}. \tag{13}$$

Then using the identity

$$\frac{1}{T+V-z} = \frac{1}{T-z}\left[1 + V\frac{1}{T-z}\right]^{-1} \tag{14}$$

one obtains for $0 < \varepsilon < \varepsilon_0$, $z \in R(d_0)$

$$\left\|D_\varepsilon \frac{1}{T+V-z}\right\| \leq 2k(d_0) \tag{15}$$

and the use of Theorem VI 5.12 from Kato's book (1966) finishes the proof of the theorem.

Remark. Even without relying on the general theorems of perturbation theory, the proof of Theorem 1 is immediate. Suppose $\varepsilon < [2k(d_0)]^{-1}$. The following formula

$$\begin{aligned} \frac{1}{T+V+\varepsilon D_\varepsilon - z} = \frac{1}{T+V-z}&\left\{\left(1 + \varepsilon D_\varepsilon \frac{1}{T+V-z_0}\right)\right. \\ &\left.\times\left[1 + \varepsilon(z_0 - z)\left(1 + \varepsilon D_\varepsilon \frac{1}{T+V-z_0}\right)^{-1} D_\varepsilon \frac{1}{T+V-z_0}\frac{1}{T+V-z}\right]\right\}^{-1} \end{aligned}$$

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

$$\left\|\varepsilon(z-z_0)\left(1 + \varepsilon D_\varepsilon \frac{1}{T+V-z_0}\right)^{-1} D_\varepsilon \frac{1}{T+V-z_0}\frac{1}{T+V-z}\right\| < 1. \tag{16}$$

In particular, if λ is the middle of a gap of magnitude ΔE then $\lambda \in \rho(H_\varepsilon)$ if

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

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

References

Borland R E 1961 *Proc. Phys. Soc.* **78** 926
Gubanov A I 1954 *Sov. Phys.-JETP* **26** 139
—— 1955 *Sov. Phys.-JETP* **28** 401
Kato T 1966 *Perturbation Theory for Linear Operators* (Berlin: Springer)
Lieb E H and Mattis D C 1966 *Mathematical Physics in One Dimension* (New York: Academic)
Mott N F and Davis J 1979 *Electronic Processes in Non-crystalline Materials* 2nd edn (Oxford: Clarendon)
Reed D and Simon B 1978 *Methods of Mathematical Physics* vol 4 (New York: Academic)