Reports of the Academy of Sciences of the USSR

PHYSICS

1966

SovietRxiv

Abstract

Full Text

Reports of the Academy of Sciences of the USSR
1966. Volume 171, No. 3

UDC 530.145

PHYSICS

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ON THE ENERGY SPECTRUM OF AN ELECTRON IN A "DEFECTIVE" ONE-DIMENSIONAL PERIODIC LATTICE

Recently a number of methods have been developed for finding the density of distribution of energy levels in disordered systems ([1–7]). One of the most important applications of these methods is the problem of determining the energy spectrum of an electron in disordered systems of the type of a "defective" lattice or amorphous bodies. Various aspects of this problem are considered in the review by I. M. Lifshits ([2]).

The main difficulty is the determination of the spectral density $\rho(E)$ near the edges of the allowed energy bands E_0, since in this case even a vanishingly small degree of disorder leads to a strong change in the character of the spectrum. In other words, the spectral density near the edge of a band behaves nonanalytically as a function of $(E - E_0)$. This leads, in particular, to the inapplicability of direct methods using an expansion in powers of the disorder ([2]).

To circumvent this difficulty in the one-dimensional case, models were found that allow asymptotic solutions to be obtained for the spectral density $\rho(E)$. In these solvable models the potential $V(x)$ in the Schrödinger equation for the electron is specified either in the form $V(x) = a \sum_k \delta(x - x_k)$, where the points x_k (the positions of the δ-like impurities) are distributed according to a random law of Poisson type ([5]), or in the form of white noise with Gaussian correlations. All these models describe completely disordered systems.

Below we shall consider a one-dimensional model of the "defective lattice" type, when the potential $V(x)$ contains a regular periodic addition $V_0(x)$ with period L_0. Thus, the initial Schrödinger equation in our model has the form:

$$\frac{d^2\Psi}{dx^2} + \left[E - V_0(x) - a\sum_k \delta(x - x_k)\right]\Psi = 0; \tag{1}$$

$$a > 0; \qquad V_0(x + L_0) = V_0(x),$$

where the coordinates of the impurity δ-functions (the points x_k) are distributed according to a Poisson law, i.e., the probability that an impurity falls in the interval $(x, x + dx)$ is equal to $\gamma\, dx$.

We shall place the impurity δ-functions at the nodes of the periodic lattice. Between two successive impurities, located at the points x_n, x_{n+1}, the solution of equation (1) has the form of Bloch wave functions, which we shall assume known:

$$\Psi_{n+1}(x) = A_{n+1} e^{iq(x-x_{n+1})} u_{n+1}(x - x_{n+1}) - A^*_{n+1} e^{-iq(x-x_{n+1})} u^*_{n+1}(x - x_{n+1}),$$

where q is the quasimomentum; $u(x)$ is a known function, periodic with period L_0. Using the continuity condition for $\Psi(x)$ and equation (1), we write–

we obtain the relation between the phases of the wave function $\Psi_n(x)$ and $\Psi_{n+1}(x)$

$$\operatorname{ctg}(\psi_{n+1} + \Delta_{n+1} - q l_n) = \operatorname{ctg}(\psi_n + \Delta_n) + \frac{a}{\operatorname{Re}\{q - iu'(0)/u(0)\}}, \tag{2}$$

where $\Delta_n = 2\pi m_n$, m_n is an arbitrary integer, with $m_{n+1} \geq m_n$; ψ_n is the phase of A_n; $l_n = x_{n+1} - x_n$ is the distance between impurity δ-functions, whose probability density is equal to

$$P(l) = \gamma e^{-\gamma l}; \qquad \gamma = 1/\langle l \rangle. \tag{3}$$

For convenience we rewrite (2) in the form

$$\operatorname{ctg}(\varphi_{n+1} - q l_n) = \operatorname{ctg}\varphi_n + \varepsilon, \tag{4}$$

where we have denoted

$$\varphi_i = \psi_i + \Delta_i; \qquad \varepsilon = a/\operatorname{Re}\{q - iu'(0)/u(0)\}; \tag{5}$$

φ_k is the phase of the wave function $\Psi(x)$ at the point x_k.

Equation (4), in its structure, is no different from the case $V_0 \equiv 0$, which makes it possible now to use the method developed in (8). In particular, for a Poisson distribution of impurities (3) we arrive at the formula obtained in (5) for the number of states $N(E)$ with energy $< E$:

$$N(E) = q \lim_{z\to-\infty} z^2 v(z); \qquad z = \operatorname{ctg}\varphi, \tag{6}$$

where $v(z)$ satisfies the equation

$$\frac{q}{\gamma}\frac{d}{dz}\left[(1+z^2)v(z)\right] = v(z) - v(z-\varepsilon), \tag{7}$$

and the normalization condition

$$\int_{-\infty}^{\infty} v(z)\, dz = 1.$$

It should be noted that in deriving equation (7) in work (8) Schmidt' s equation (4) was used,

$$w(\varphi_{n+1}) = \int w(\varphi_n)\frac{d\varphi_n}{d\varphi_{n+1}} P(l_n)\, dl_n, \tag{8}$$

where $w(\varphi)$ is the normalized distribution function of the phase φ, while the relation between φ_n, φ_{n+1}, and l_n is determined by relation (4). In our case l_n takes a discrete series of values, multiples of the lattice period L_0, and the transition in (8) to integration instead of summation can be made if the impurities are rare: $\langle l\rangle \gg L_0$.

Thus, the problem under consideration is reduced to the case of absence of the periodic part in the potential by means of a definite renormalization: replacing k in (7) by q and using the expression for ε modified according to (5). It is obvious that these changes do not, generally speaking, reduce simply to the trivial introduction of an effective electron mass in (1).

In the case when $V_0 \equiv 0$, we have

$$q = k, \qquad \varepsilon = a/k \quad (k^2 = E), \tag{9}$$

and equation (7) coincides with that considered in (8) in the absence of a periodic field. In this limit the boundary of the spectrum corresponds to $k = 0$, and the density of states for $k \to 0$, found in (8), has the form:

$$\rho(E) \sim E^{-3/2} \exp\{-\pi\gamma/\sqrt{E} + \alpha'\gamma/a\} \qquad (\alpha \sim 1). \tag{10}$$

For $V_0 \neq 0$ we can use the known solution of equation (7), using the form of q and ε for a concrete periodic potential. As an example, let us consider the Kronig–Penney model:

$$V_0(x) = a_0 \sum_n \delta(x - nL_0); \qquad a > 0; \qquad n = 0, \pm 1, \ldots$$

In this case

$$u(x) = e^{i(k-q)x} + Be^{-i(k+q)x}, \qquad B = (1 - e^{i(k-q)L_0})/(e^{-i(k+q)L_0} - 1), \quad (11)$$

$$\varepsilon = \frac{a}{k}\frac{\sin kL_0}{\sin qL_0}; \qquad \cos qL_0 = \cos kL_0 + \frac{a_0}{2k}\sin kL_0.$$

Near the left edge E_0, for the first allowed band, it follows from (11) that

$$q \approx \sqrt{E - E_0}; \qquad \varepsilon \approx a/\sqrt{E - E_0}. \quad (12)$$

Making the corresponding substitutions in (10), according to (9), we find

$$\rho(E) \sim (E - E_0)^{-3/2} \exp\{-\pi\gamma/\sqrt{E - E_0} + a\sqrt{\gamma/a}\}. \quad (13)$$

Near the right edge of the band E_1, $q \to \pi/L_0$, $\varepsilon \to 0$. For energies E sufficiently close to E_1, the inequality $\gamma\varepsilon/q \ll 1$ is always satisfied. This makes it possible to expand $v(z - \varepsilon)$ in equation (7) in a series in ε and to retain only the first two terms of the expansion:

$$\frac{q}{\gamma}\frac{d}{dz}\left[(1 + z^2)v(z)\right] = \varepsilon\frac{dv(z)}{dz}. \quad (14)$$

Equation (14) is immediately integrated and, in accordance with (6), gives

$$\rho(E) = \frac{dN(E)}{dE} \approx \frac{1}{2\pi}\sqrt{\frac{a_0 L_0}{2}}\,(E_1 - E)^{-1/2}, \quad (15)$$

i.e., the usual square-root singularity is preserved, as in the absence of impurities. Figure 1 shows the curves $\rho(E)$ in the case without impurities (dashed line) and in the presence of impurities (solid line). The result obtained is easy to understand, since the character of the random impurities chosen by us shifts the left boundary of the allowed energy band to the right and thereby smears the boundary, whereas the position of the right boundary does not depend on the impurities. The forbidden regions do not change in the case under consideration. Near the edge of the n-th band, in formulas (13), (15), $E_{0,1}$ should be replaced by E_n.

Fig. 1

Fig. 2

Fig. 1 and Fig. 2: schematic plots of $\rho(E)$ versus E, with dashed and solid curves; energy levels marked E_0, E_1 in Fig. 1 and E_0, E_1, E_2, E_3 in Fig. 2.

Figure 1: Fig. 1 and Fig. 2: schematic plots of $\rho(E)$ versus E, with dashed and solid curves; energy levels marked E_0, E_1 in Fig. 1 and E_0, E_1, E_2, E_3 in Fig. 2.

An analogous solution can be carried out for any periodic potential $V_0(x)$, using its specific form to determine q and ε instead of formulas (11).

The method of renormalizing the basic parameters q and ε in order to preserve the relation between the phases of wave functions of type (4) can also be used for another limiting case—very large impurity concentrations $\langle l \rangle \ll L_0$. Let, for example, the impurity potential $V(x)$ be Gaussian "white noise" :

$$\langle V(x) \rangle = 0; \qquad \langle V(x)V(x') \rangle = \sigma^2 \delta(x - x'). \tag{16}$$

The random field (16) can be represented in the form (9)

$$V(x) = \sum_k a_k \delta(x - x_k), \tag{17}$$

where $a_k = \pm a$ $(a > 0)$, each with probability 1/2, while the points x_k are still distributed according to the Poisson law with parameter γ, and distribution (16) is obtained in the limit:

$$a \to 0, \qquad \gamma \to \infty, \qquad \gamma a^2 = \text{const} = \frac{1}{2}\sigma^2. \tag{18}$$

In paper ([8]) it was shown that formula (6) is also preserved in the case of (17), while the equation for $v(z)$ has, for $V_0 \equiv 0$, the form

$$\frac{k}{\gamma}\frac{d}{dz}\left[(1+z^2)v(z)\right] = v(z) - \frac{1}{2}v(z-\varepsilon) - \frac{1}{2}v(z+\varepsilon) \qquad \left(\varepsilon = \frac{a}{k}\right), \tag{19}$$

whence, with the aid of the limiting transition (18) and (6), the result of paper ([7]) follows:

$$N(E) = \pi^{-2}\left\{\left[\mathrm{Ai}\left(-\frac{k^2}{(\sigma^2/2)^{2/3}}\right)\right]^2 + \left[\mathrm{Bi}\left(-\frac{k^2}{(\sigma^2/2)^{2/3}}\right)\right]^2\right\}^{-1}, \tag{20}$$

where Ai, Bi are Airy functions. Formula (6) follows ([8]) from

$$N(E) = \frac{1}{\pi}\sum_{k=1}^{M}\langle \Delta\varphi_k \rangle = \frac{1}{\pi}\sum_{k=1}^{M}\langle \varphi_k - \varphi_{k-1} \rangle, \tag{21}$$

where M is the number of δ-functions along the length of the lattice, and the averaging is carried out over all configurations. Let us use the fact that the mean distance between impurities, according to (18), tends to zero. Then it is not difficult to obtain:

$$N(E) = \frac{1}{L_0}\int_0^{L_0} dx\, N(E,x) = \frac{1}{\pi L_0}\int_0^{L_0} dx\, \langle \Delta\varphi_k(x)\rangle, \qquad (22)$$

where $N(E,x)$ is calculated with the aid of equations (19), (6), in which the parameter $\varepsilon = \varepsilon(x)$. For the Kronig–Penney model, according to (11), we have

$$N(E,x) = \pi^{-2}\{[\mathrm{Ai}(-\xi)]^2 + [\mathrm{Bi}(-\xi)]^2\}^{-1}, \qquad (23)$$

$$\xi = \left[\frac{2}{\sigma^2}\, qk^2\, \frac{\sin^2 kL_0 \cdot \sin^2 qL_0}{f^2(x)}\right]^{2/3},$$

$$f(x) = \sin^2 kx \cdot \sin^2 qL_0 + [\sin k(L_0 - x) + \sin kx \cdot \cos qL_0]^2.$$

In particular, for $V_0 \equiv 0$ we have $\xi = k^2(2/\sigma^2)^{2/3}$, and (20) follows at once from (22). Omitting the cumbersome investigation of formula (23), which solves the problem in principle, we arrive at $\rho(E)$, having qualitatively the form shown in Fig. 2 (the notation is the same as in Fig. 1).

In conclusion we note that if, in the case of the Poisson distribution of impurities (3), the latter are placed not at the lattice sites, then the right edge of the allowed band is shifted to the right and the singularity near the right edge of the band is smeared out. This fact is easily established by using the corresponding value of $\varepsilon(x)$.

Received
3 V 1966

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Note: Figure translations are in progress. See original paper for figures.