

SHAPE OF THE ELECTRON ENERGY SPECTRUM FOR A ONE-DIMENSIONAL RANDOM LATTICE

L. I. MAGARILL and M. V. ÉNTIN

Submitted to JETP editor June 23, 1966

J. Exptl. Theoret. Phys. (U.S.S.R.) 51, 1852-1855 (December, 1966)

The energy spectrum of an electron in a one-dimensional system of randomly distributed potential centers is investigated under the assumption of a Poisson distance distribution and smallness of the product of the potential and mean distance between the centers.

WE investigate in this paper the energy spectrum of an electron in a one-dimensional system of randomly distributed potential centers. The potential energy of the electron in such a system is

$$U(x) = a \sum_k \delta(x - x_k).$$

We assume a Poisson distribution of the distances between centers. The case  $a < 0$  was considered by Frish and Lloyd<sup>[1]</sup>, who determined the density of the number of levels by numerical methods, and who also obtained formulas for several limiting cases. However, for no region of the parameters characterizing the potential ( $a, \bar{l} = \overline{x_k - x_{k-1}}$ ) was an analytic expression obtained for the level density in the entire energy region. Bychkov and Dykhne<sup>[2]</sup> discussed the case  $a\bar{l} \gg 1, a < 0$ . The structure of the impurity band for  $|a\bar{l}| \gg 1, a > 0$  was considered by I. Lifshitz<sup>[3]</sup>. Zaslavskii and Pokrovskii<sup>[4]</sup> investigated the case  $a\bar{l} \ll 1, a > 0, k^2 \ll a/\bar{l}$ , where  $k^2 = E$  is the electron energy. We shall assume that  $|a\bar{l}| \ll 1$ , but will impose no limitations whatever on the energy.

Let us clarify the physical difference between the cases  $|a\bar{l}| \gg 1$  and  $|a\bar{l}| \ll 1$ . When  $|a\bar{l}| \gg 1$  the two neighboring  $\delta$ -functions, separated by a distance on the order of  $\bar{l}$ , form an effective potential well with rigid walls. In our case, however, no level can arise between two neighboring  $\delta$ -functions separated by a distance on the order of  $\bar{l}$ . Indeed, with respect to the uncertainty we have for the very first level  $k \sim 1/\bar{l}$ , and the coefficient of reflection from the  $\delta$ -function is of the order of  $|a/k| \ll 1$ . Consequently, an important role is played in this case by multiple scattering.

The characteristic energy for  $|a\bar{l}| \ll 1$  is  $a/\bar{l}$ , in the vicinity of which the density of the number of levels is maximal. The energy  $1/\bar{l}^2$ , which is characteristic when  $|a\bar{l}| \gg 1$ , does not play any role at all in our case.

We consider first the case  $a > 0$  (repulsive potential). Zaslavskii and Pokrovskii<sup>[4]</sup> have shown that the number of levels with energy smaller than  $E$  is expressed in terms of the auxiliary function  $V(z)$ :

$$N(E) = k \lim_{z \rightarrow \infty} z^2 V(z). \tag{1}$$

The function  $V(z)$  satisfies the equation

$$\frac{1}{\gamma} \frac{d}{dz} [(z^2 + 1)V(z)] = V(z) - V(z - \epsilon), \quad \gamma = \frac{1}{k\bar{l}}, \quad \epsilon = \frac{a}{k} \tag{2}$$

and the normalization condition

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

Our notation is the same as in<sup>[4]</sup>. Equation (2) is solved by a method analogous to that used here.

We can separate three main energy regions:

1.  $E > E_0 = a/\bar{l}$ ,  $(E - E_0)/E_0 \gg (a\bar{l})^{1/3}$ . Here  $V(z)$  has the following form:

$$V(z) = \frac{1}{2\pi} \frac{\sqrt{1 - E_0/E}}{z^2 + 1 - E_0/E}.$$

We see therefore that the "average potential" approximation is valid, and

$$N(E) = \sqrt{E - E_0} / 2\pi. \tag{3}$$

2.  $|E - E_0|/E_0 \ll 1$ . In this region the solution of (2) can be obtained by expanding  $V(z - \epsilon)$  in powers of  $\epsilon$  and retaining terms of order  $\epsilon^2$ . Retaining in the solution the part that is bounded at  $-\infty$ , we have

$$V(z) = B \exp[\Phi(z)] \int_{-\infty}^z \exp[-\Phi(z')] dz', \tag{4}$$

where

$$\Phi(z) = \frac{2}{\gamma \epsilon^2} \left( z_0^2 z - \frac{z^3}{3} \right), \quad z_0^2 = \frac{E_0}{E} - 1$$

(in the case when  $E_0/E < 1$ , the quantity  $z_0$  is imaginary).

The coefficient B is determined from the normalization. Calculating the normalization integral, we obtain

$$N(E) = k \sqrt{\frac{\gamma \epsilon^2}{8\pi}} \left\{ \int_0^\infty \frac{d\xi}{\sqrt{\xi}} \exp \left[ \frac{2}{\gamma \epsilon^2} \left( z_0^2 \xi - \frac{\xi^3}{12} \right) \right] \right\}^{-1}. \quad (5)$$

When  $(E_0 - E)/E_0 \gg (a\bar{l})^{1/3}$  and  $(E_0 - E)/E_0 \ll 1$  ( $z_0^2 \gg (\gamma \epsilon^2)^{2/3}$ ,  $z_0 \ll 1$ ), we get for  $N(E)$  from (5)

$$N(E) = \frac{1}{2\pi} \sqrt{E_0 - E} \exp \left\{ -\frac{8}{3} \frac{(E_0 - E)^{3/2}}{aE_0} \right\}. \quad (6)$$

When  $(E_0 - E)/E_0 \gg (a\bar{l})^{1/3}$ , Eq. (5) yields

$$N(E) = \frac{6^{5/6}}{2^{7/2} \sqrt{\pi} \Gamma(1/6)} (aE_0)^{1/3} \left[ 1 - \frac{\sqrt{2\pi/3} (E_0 - E)}{\Gamma(1/6) (aE_0)^{2/3}} \right]. \quad (7)$$

3.  $(E_0 - E)/E_0 \gg (a\bar{l})^{1/3}$ . Without repeating the calculations of [4], we note only the main steps. In the regions  $|z \pm z_0| \ll \gamma \epsilon / z_0$ , the function  $V(z - \epsilon)$  can be expanded in powers of  $\epsilon$ . In the region  $|z \pm z_0| \gg \sqrt{\gamma^2 / z_0}$  we can use the WKB method. Joining together the solutions obtained in the regions  $\sqrt{\gamma \epsilon^2 / z_0} \gg |z \pm z_0| \gg \gamma \epsilon / z_0$  and normalizing  $V(z)$  to unity, we obtain, using (1),

$$N(E) = \frac{1}{2\pi} \sqrt{E_0 - E} \exp \left\{ -\frac{2}{k\bar{l}} \operatorname{arctg} \sqrt{\frac{E_0}{E} - 1} - \frac{1}{\sqrt{a\bar{l}}} \int_{E/E_0}^1 \left[ u(t) - \frac{1}{t} \right] \frac{dt}{\sqrt{t - E/E_0}} \right\}, \quad (8)$$

where  $u(t)$  is determined by the equation  $tu(t) = 1 - \exp[-u(t)]$ .

When  $E \ll E_0$ , Eq. (8) goes over into the results of Zaslavskii and Pokrovskii [4].

Let us write out the explicit form of the function  $V(z)$ . In the region  $|z + z_0| \ll \gamma \epsilon / z_0$ , the function  $V(z)$  can be represented in the form

$$V(z) = A \exp[\Phi(z)] \int_{-\infty}^z \exp[-\Phi(z')] dz',$$

where

$$A = \frac{4z_0}{\gamma \epsilon^2} \exp \left\{ -\sqrt{\frac{1}{a\bar{l}}} \int_{E/E_0}^1 u(t) \frac{dt}{\sqrt{t - E/E_0}} \right\}.$$

In the region  $z_0 > z > -z_0$ ,  $|z \pm z_0| \gg \sqrt{\gamma \epsilon^2 / z_0}$ , we have

$$V(z) = \sqrt{\frac{2z_0}{\pi \gamma \epsilon^2}} \exp \left\{ \sqrt{\frac{1}{a\bar{l}}} \int_{-z_0/\sqrt{\gamma \epsilon}}^{z_0/\sqrt{\gamma \epsilon}} u \left( x^2 + \frac{E}{E_0} \right) dx \right\}.$$

Finally, in the region  $|z - z_0| \ll \gamma \epsilon / z_0$

$$V(z) = \exp \{ \Phi(z) \} \left[ \sqrt{\frac{2z_0}{\pi \gamma \epsilon^2}} e^{-4z_0^3/3\gamma \epsilon^2} + A \int_{z_0}^z \exp \{ -\Phi(z') \} dz' \right].$$

Regions 1, 2, and 3 overlap, and the corresponding formulas go over into one another at the intersections of these regions.

Let us consider the case  $a < 0$ . Now the electron energy can be negative. Frish and Lloyd [1] obtain an equation for the distribution function  $V(z)$  of the quantity  $z = \psi' / |k|\psi$ , where  $\psi$  is the wave function. For  $E > 0$  the equation for  $V(z)$  coincides with (2) if we replace  $\epsilon$  by  $-\epsilon$ , and takes for  $E < 0$  the form

$$\frac{1}{\gamma} \frac{d}{dz} [V(z)(z^2 - 1)] = V(z) - V(z + \epsilon),$$

where now  $\gamma = 1/|k|\bar{l}$  and  $\epsilon = |a/k|$ . In formula (1) for the number of levels,  $k$  should be replaced by  $|k|$ .

In analogy with the preceding, we find that in the region  $(E - E_0)/|E_0| \gg (|a|\bar{l})^{1/3}$  formula (3) remains valid as before. In the region  $|E - E_0|/|E_0| \ll 1$ , formula (5) is valid if  $z_0^2$  is taken to mean the quantity  $1 - \gamma \epsilon$ . In the region  $(E_0 - E)/E_0 \gg (|a|\bar{l})^{1/3}$  we have

$$N(E) = \frac{1}{2\pi} \sqrt{E_0 - E} \exp \left\{ \frac{1}{\sqrt{|a|\bar{l}}} \int_1^{E/E_0} u(t) \frac{dt}{\sqrt{E/E_0 - t}} \right\}, \quad (9)$$

where  $u(t)$  has the same meaning as before.

For large negative  $E$  we obtain from (9)

$$N(E) \sim \sqrt{-E} \exp \left\{ -2 \frac{\sqrt{-E}}{|a|} \ln \left( \frac{E}{E_0} \right) \right\}. \quad (10)$$

We have used the fact that at large values of  $t$  the function  $u(t) \sim -\ln t$ . The latter result corresponds physically to a situation wherein a large number of  $\delta$ -functions is gathered within a length of the order of  $|E|^{-1/2}$ , forming a deep potential well in which the lower energy level is equal to  $E$ .

In conclusion, we are deeply grateful to V. L. Pokrovskii for guidance of this work.

<sup>1</sup>H. L. Frish and S. P. Lloyd, Phys. Rev. **120**, 1175 (1960).

<sup>2</sup>Yu. A. Bychkov and A. M. Dykhne, JETP Letters **3**, 313 (1966), transl. p. 202.

<sup>3</sup>I. M. Lifshitz, JETP **44**, 1723 (1963), Soviet Phys. JETP **17**, 1159 (1963).

<sup>4</sup>G. M. Zaslavskii and V. L. Pokrovskii, JETP **51**, 449 (1966), Soviet Phys. JETP **24**, 303 (1967).