ELECTRON ENERGY SPECTRUM IN A ONE-DIMENSIONAL FLUID MODEL

G. M. ZASLAVSKIĬ and V. L. POKROVSKIĬ

Novosibirsk State University

Submitted to JETP editor January 18, 1966

J. Exptl. Theoret. Phys. (U.S.S.R.) 51, 449–461 (August, 1966).

The energy spectrum of an electron in a one-dimensional completely-disordered system is studied. The lattice points are approximated by δ-like potential barriers. The distance between the points is a random function. The density of the probability of the distance between the points is assumed to be an exponentially decreasing function of the distance. A method is developed for obtaining an asymptotically exact expression for the density of the energy spectrum near the edge of the energy band.

THE question of the structure of the energy spectrum of electrons in a liquid (liquid metal, dielectric, etc.) is of interest in physics. Unfortunately, great mathematical difficulties arise in its solution, and it is sensible to investigate the simplest one-dimensional model. Hopes are raised, in particular, by the fact that the spectrum of the one-dimensional model of the crystal has the same basic features as the spectrum of a real solid (band structure, especially at the edges of the bands). This apparently explains why a large number of papers have been devoted to one-dimensional systems. Dyson's pioneering paper[1] deals with the spectrum of a one-dimensional chain of coupled oscillators. The connection between this problem and the problem of the electron spectrum is well known. An extensive literature is also devoted to the influence of small distortions of the crystal lattice (or oscillator chain) on the spectrum (see the papers of I. Lifshitz,[2] Montroll and Potts,[3] and Schmidt[4]).

In the investigation of the one-dimensional model of a liquid there are in fact two meaningful questions: 1) How is the discrete level spread out into a narrow band (this question, naturally, is meaningful when the distance between lattice points is larger than the radius of the bound states)? 2) What is the structure of the edge of the energy band? The first question was investigated in the one-dimensional case by Frish and Lloyd,[5] and in the three-dimensional case by I. Lifshitz.[2] It must be noted that both the first and second question were investigated by I. Lifshitz[2] with exponential accuracy for a great variety of situations and for an arbitrary number of dimensions.

The main idea consists in the following. Let, for example, the points of the "lattice" be randomly distributed potential barriers. To realize a state with an energy much lower than the average potential energy of the barriers it is necessary, in accordance with the uncertainty relation, that the neighboring lattice points be moved apart by a distance of half wavelength $\lambda/2$. For large λ such a configuration has low probability, and an estimate of the density of the energy spectrum reduces to an estimate of the probability of such a fluctuation. No account is taken here, however, of the quantum effect of the penetration of the particles into the potential barrier. In this paper we consider a situation in which this effect is essential, and find an asymptotically exact expression for the energy spectrum.

We represent the one-dimensional liquid by a model of randomly arranged potential centers, from which the electrons are scattered. For simplicity, the dimension of the potential centers is assumed much smaller than the electron wavelength and the average distance between centers. Such assumptions allow us to write for the potential

$$V(x) = a\sum_k \delta(x - x_k); \qquad a > 0.$$

The interaction between the potential centers x_k is taken into account in very simple fashion by specifying the distribution functions $P(l_k)$ of the distances $l_k = x_{k+1} - x_k$ between centers. In such a formulation, the edge of the band corresponds to the region of small values of k.

1. BASIC EQUATIONS AND SOME GENERAL RELATIONS

Our problem is to find the average level density of the Schrödinger equation

$$\frac{d^2\Psi}{dx^2}+\left[k^2-a\sum_i\delta(x-x_i)\right]\Psi=0 \qquad (1.1)$$

with boundary conditions

$$\Psi(0)=\Psi(x_{M+1})=0 \qquad (1.2)$$

for a specified distribution $P(l)$ of the distance l between two nearest lattice points. Averaging over all possible configurations $\{x_k\}$ is understood. Owing to ergodicity, the average level density defined in this manner coincides with the level density of a sufficiently long chain. Solution of (1.1) in the interval (x_n, x_{n+1}) is of the form

$$\Psi_{n+1}(x)=A_{n+1}\sin\left[k(x-x_{n+1})+\psi_{n+1}\right], \qquad (1.3)$$

the connection between phases ψ_n and ψ_{n+1} being given by

$$\operatorname{ctg}(\psi_{n+1}-l_n)=\operatorname{ctg}\psi_n+\varepsilon, \qquad (1.4)^*$$

where

$$l_n=k(x_{n+1}-x_n),\quad \varepsilon=a/k. \qquad (1.5)$$

Usually one considers a system of length L with subsequent transition to $L\to\infty$. We, on the other hand, consider a system with a specified number of points M + 1. These problems are physically equivalent, for with a very high degree of accuracy, in accord with the law of large numbers, the length of the chains is for the overwhelming majority of configurations,

$$L=M\bar{l}=M/\gamma,\quad L,M\to\infty, \qquad (1.6)$$

where $\bar{l}\equiv\gamma^{-1}$ is the average distance between lattice points multiplied by k (see (1.5)).

The number of states $N_L(E)=N_L(k^2)$ with energy lower than E is equal to the number of zeroes of the wave function in a length L. Each possible placement of the δ functions (i.e., of the points x_i) over a length L defines a configuration Γ and a corresponding number of states $N_L(E,\Gamma)$. The number of levels with energies smaller than E, averaged over all the configurations Γ and taken per unit length, is

$$N(E)=\lim_{L\to\infty}\frac{1}{L}\overline{N_L(E,\Gamma)}, \qquad (1.7)$$

where the bar denotes averaging over the configurations. Schmidt has shown[4] that N(E) has a finite limit and can be represented in the form

$$N(E)=\pi^{-1}\gamma\langle\psi_{n+1}(\psi_n)-\psi_n\rangle, \qquad (1.8)$$

where the angle brackets denote averaging over the distribution function $W(\psi_n)$ of the phase ψ_n.

*ctg ≡ cot.

Formula (1.8) is a result of the following reasoning. In our notation, the phase of the wave function at the end of an interval of length L, on which are located M atoms with δ-function potential, is ψ_{M+1}. It follows from the boundary conditions (1.2) that $\psi_{M+1}=m\pi$. If we agree that

$$|\psi_{n+1}-l_n-\psi_n|<\pi,$$

then the number m is indeed the number of the level for the given configuration. The number of states $N_L(E,\Gamma)$, which naturally depends on the configuration Γ and on the length of the interval, is

$$N_L(E,\Gamma)=\frac{1}{\pi}\psi_{M+1}\equiv\frac{1}{\pi}\sum_{k=0}^{M}(\psi_{k+1}-\psi_k),$$

with $\psi_{k+1}=\psi_{k+1}(\psi_k, l_k, E)$. As $M\to\infty$ we can write, in accord with the law of large numbers,

$$N_L(E,\Gamma)\approx\pi^{-1}M\langle\psi_{k+1}(\psi_k,l_k,E)-\psi_k\rangle.$$

where the angle brackets have the same meaning as in (1.8). Averaging the resultant expression over all the configurations Γ (i.e., over l_k), we obtain after dividing by L the average number of levels per unit length:

$$N(E)=\frac{M}{\pi L}\langle\overline{\psi_{k+1}(\psi_k,l_k,E)-\psi_k}\rangle.$$

If we now recall the notation in (1.6), then we arrive in the limit at formula (1.8). Actually, we have already assumed in the derivation that the distribution $W(\psi_n)$ reaches a stationary value, if ψ_n is regarded as a coordinate on a circle, and therefore we must assume that n in (1.8) is sufficiently large. The main difficulty in determining the number of energy levels is transferred in such an approach to the determination of the phase distribution function $W(\psi)$.

Let us write the probability that on the n-th step (i.e., after passing through n δ functions) the phase ψ_n lies in the interval $(\psi_n, \psi_n+d\psi_n)$, in the form of the Smoluchowski integral equation

$$W_n(\psi_n)\,d\psi_n=\int W_{n-1}[\psi_{n-1}(\psi_n,l_n)]\,d[\psi_{n-1}(\psi_n,l_n)]P(l_n)\,dl_n. \qquad (1.9)$$

The connection between the phases ψ_{n-1} and ψ_n in (1.9) is determined by the condition (1.4). For sufficiently large n, when $W_n(\psi_n)$ tends to its stationary value that does not depend on n, we obtain the integro-functional equation:[4]

$$W(\psi)=\int dl\,W[\psi'(\psi,l)]\frac{d\psi'(\psi,l)}{d\psi}P(l),$$
$$\operatorname{ctg}(\psi-l)=\operatorname{ctg}\psi'+\varepsilon. \qquad (1.10)$$

The solution of (1.10) should be periodic with period π, non-negative, and satisfying the normalization condition

$$\int_0^{\pi} W(\psi)\,d\psi = 1.$$

There is one more simple relation, besides (1.8), between the number of levels and the distribution functions $W(\psi)$ and $P(l)$. This relation is based on a direct count of the average number of zeroes of the wave function in the interval between two lattice points:

$$N(E) = \sum_{n=1}^{\infty} n \int_{n\pi}^{(n+1)\pi} d\eta \int_0^{\pi} d\eta \int_0^{\infty} dl\, W(\eta + l) P(l) P(\psi - \eta).$$

For some particular types of the distribution $P(l)$, the Schmidt equation (1.10) can be reduced to a differential-difference equation. Let the probability that the distance between two δ functions lies in the interval $(l, l + dl)$ be equal to

$$P(l)\,dl = \gamma e^{-\gamma l} dl, \tag{1.11}$$

which corresponds to a Poisson distribution of the points x_y in the Schrödinger equation (1.1). Differentiation of (1.10) with respect to ψ yields

$$\frac{1}{\gamma}\frac{dW(\psi)}{d\psi} = W[\psi'(\psi)]\frac{d\psi'(\psi)}{d\psi} - W(\psi), \tag{1.12}$$

where

$$\operatorname{ctg}\psi'(\psi) = \operatorname{ctg}\psi - \varepsilon, \tag{1.13}$$

or, introducing

$$\operatorname{ctg}\psi = z, \quad V(z)\,dz = W(\psi)\,d\psi, \quad \int_{-\infty}^{\infty} V(z)\,dz = 1, \tag{1.14}$$

we have[1)]

$$\frac{1}{\gamma}\frac{d}{dz}[(1+z^2)V(z)] = V(z) - V(z-\varepsilon). \tag{1.15}$$

Similarly, for distributions $P(l)$ of the type

$$P(l) = A\sum_{k=1}^{n} e^{-\gamma_k l}, \quad P(l) = A l^n e^{-\gamma l} \tag{1.16}$$

we can obtain for $W(\psi)$ an n-th order differential equation with shifted arguments.

In Appendix 1 we shall obtain a differential equation and a solution by the method described above for the case when the potential V(x) in the Schrödinger equation has a Gaussian distribution.

We proceed now to investigate formula (1.8) for the number of states. Frish and Lloyd[5] obtained by the Rice method[6] for N(E), in the case of a Poisson distribution of the δ functions,

$$N(E) = \lim_{z\to\pm\infty} z^2 V(z). \tag{1.17}$$

The result (1.17) is quite remarkable, since it makes it possible to find immediately, once the phase distribution function $W(\psi)$ has been obtained, the number of states without any additional averaging operations, as would be necessary if (1.8) were used. We shall show the connection between (1.8) and (1.17) later. Actually formula (1.17) is not valid for arbitrary distributions of the distances between atoms, but for certain types of the distribution $P(l)$ we can express the number of levels N(E) in terms of V(z) and derivatives of V(z) as $z \to \pm\infty$, bypassing the inconvenient averaging operation in (1.8).

From the second equation in (1.10) we get

$$\Delta\psi = \psi - \psi' = l + \operatorname{arcctg}[\operatorname{ctg}\psi' + \varepsilon] - \psi'$$
$$= l + \operatorname{arcctg}[z + \varepsilon] - \operatorname{arcctg} z, \quad z = \operatorname{ctg}\psi'. \tag{1.18}*$$

Hence, in accord with (1.8), we obtain

$$N(E) = \frac{1}{\pi}\gamma\langle\overline{\Delta\psi}\rangle = \frac{1}{\pi}\gamma\int_0^{\infty} P(l)\,dl$$
$$+ \frac{1}{\pi}\gamma\int_{-\infty}^{\infty} V(z)\{\operatorname{arcctg}(z+\varepsilon) - \operatorname{arcctg} z\}\,dz$$

or, after making a change of variable in the second integral and recognizing that γ^{-1} is precisely the average distance between neighboring δ functions;

$$N(E) = \frac{1}{\pi} + \frac{1}{\pi}\gamma\int_{-\infty} \operatorname{arcctg} z\{V(z-\varepsilon) - V(z)\}\,dz. \tag{1.19}$$

In the case of a Poisson distribution of $P(l)$ we get from (1.19), using (1.15),

$$N(E) = \lim_{z\to-\infty} z^2 V(z)$$

and we arrive at the result (1.17).

We can similarly obtain convenient expressions for N(E) for certain other types of distributions of distances between δ functions (see Appendix 2).

2. POISSON DISTRIBUTION

In order not to clutter up the main outline of the solution with excessive details, we present the solution using a concrete example with a distribution

$$P(l) = \bar{l}^{-1} e^{-l/\bar{l}}, \tag{2.1}$$

for which the main integral equation (1.10) reduces to the differential-difference equation (1.15). Unfortunately, we cannot present the solution of (1.15)

[1)] This differential equation was obtained by Frish and Lloyd[5] in a different manner and was investigated for the case $\epsilon < 0$.

*arcctg $\equiv \cot^{-1}$.

in explicit form. The most trivial approximate solution is the solution in the case when $\epsilon \ll 1$ and $\gamma\epsilon \ll 1$. It is obtained by expanding the right side of (1.15) in a series in ϵ up to the first derivative inclusive, and takes the form

$$W(\psi) = C / (1 - \gamma\varepsilon \sin^2 \psi). \quad (2.2)$$

The solution (2.2) has been purposely written with exaggerated accuracy, since it is valid in this form even when perturbation theory is not applicable ($\epsilon \ll 1$, $\gamma\epsilon < 1$). If $\gamma\epsilon > 1$, a pole appears formally in the solution (2.2), indicating that (2.2) is not valid in a certain angle interval. We shall discuss in detail only the case $\gamma\epsilon \gg 1$, corresponding to the bottom of the band.

We shall preface the exact solution by a heuristic analysis. It follows from (1.10) that for any ψ_n which is not small, and for small $\bar{l}$, the value of ψ_{n+1} is with overwhelming probability smaller than ψ_n. Therefore, even if as a result of a low-probability fluctuation the angle ψ turns out to be not small, after several steps it will "roll down" into the region of small ψ. For small ψ, formula (1.10) can be written approximately in the form

$$\psi' - \psi = kl - \varepsilon\psi^2. \quad (2.3)$$

It follows from (2.3) that in the vicinity of the point $\psi_0 = (k\bar{l}/\epsilon)^{1/2}$ disordered diffuse motion of the phase takes place and causes ψ_0 to become the point of the maximum of the distribution $W(\psi)$. We are justified in expecting that in the main the phase points on the circle will be concentrated around the small $\psi_0 = (\bar{l}k/\epsilon)^{1/2}$. The occurrence of the level corresponds to low-probability phase jumps by π (and larger), connected with the large intervals l ($kl > \pi$). From the condition (1.14) and from Eq. (1.15) it follows that the limits $\lim z^2V(z)$ as $z \to -\infty$ and $z \to +\infty$ coincide, which, incidentally, is obvious, since these limits have the meaning of $W(0)$. The maximum of $V(z)$ lies at the point $z_0 = \sqrt{\gamma\epsilon} \gg 1$.

We shall start the investigation of the solution $V(z)$ from the vicinity of the point of the maximum. It is to be expected that $V(z - \epsilon)$ can be expanded in the vicinity of this point in a series in ϵ. since a function varies weakly in the vicinity of an extremum. In this approximation, Eq. (1.15) takes the form

$$^1/_2\gamma\varepsilon^2V''(z) + (z^2 - \gamma\varepsilon)V'(z) + 2zV(z) = 0 \quad (2.4)$$

(we neglect unity compared with z^2). Equation (2.4) has a general solution in the form

$$V(z) = e^{\xi(z)}\left\{A_+ + B_+\int_{z_0}^{z} e^{-\xi(z)}\,dz\right\},$$

$$\xi(z) \equiv \frac{2}{\gamma\varepsilon^2}\left(\gamma\varepsilon z - \frac{z^3}{3}\right), \quad (2.5)$$

where A_+ and B_+ are arbitrary constants. The first term corresponds to the expected sharp maximum of width $|z - z_0| \sim \gamma^{1/4}\epsilon^{3/4}$, and behaves approximately like $\exp[-\alpha(z - z_0)^2]$. The second term reverses sign at the point z_0 and behaves when $|z - z_0| \gg \gamma^{1/4}\epsilon^{3/4}$ like $(z^2 - \gamma\epsilon)^{-1}$, so that the constant A_+ should be sufficiently large and positive. The condition for the solution (2.4) to be expandable in a series in ϵ is satisfied in the region

$$|z - z_0| \ll \sqrt{\gamma\varepsilon}. \quad (2.6)$$

A similar solution can be obtained in the vicinity of the point $-z_0$, but here we write it for convenience in the form

$$V(z) = e^{\xi(z)}\left(A_- + B_-\int_{-\infty}^{z} e^{-\xi(z)}dz\right), \quad |z + z_0| \ll \sqrt{\gamma\varepsilon}. \quad (2.7)$$

The integration in the right side of (2.7) is carried out formally in the region where the solution (2.7) is not valid. Actually, however, the integrand has a sharp maximum at the point $-z_0$, with a width $|z + z_0| \sim \gamma^{1/4}\epsilon^{3/4}$, so that the main contribution to the integral is made by the "legitimate" region $|z + z_0| \ll \sqrt{\gamma\epsilon}$. In the solution (2.7), the first term corresponds to an exponential function that increases on both sides of the point $-z_0$, approximately like $\exp[\alpha(z + z_0)^2]$, while the second behaves in somewhat more complicated fashion: when $z_0 - z \gg \gamma^{1/4}\epsilon^{3/4}$ it can be approximated by the quantity $^1/_2\gamma\epsilon^2B_-(z^2 - \gamma\epsilon)^{-1}$, and when $z - z_0 \gg \gamma^{1/4}\epsilon^{3/4}$, by the quantity

$$V(z) \approx \frac{1}{2}\sqrt{\pi}\,\gamma^{1/4}\varepsilon^{3/4}B_-\exp\left\{-\frac{4}{3}\sqrt{\frac{\gamma}{\varepsilon}} + \xi(z)\right\}. \quad (2.8)$$

To determine the form assumed by the solutions of the type $A\exp\{\xi(z)\}$ outside the intervals $|z \pm z_0| \ll \sqrt{\gamma\epsilon}$ we use a modified WKB method. We seek the solution in the form

$$V(z) = e^{S(z)}. \quad (2.9)$$

The meaning of this notation is that we assume that in general we cannot represent the quantity $V(z - \epsilon)$ in the form of a series in powers of ϵ and then retain only a few terms, whereas for $S(z)$ this is permissible. Accepting this assumption and confining ourselves to only two terms in the expansion of $S(z)$ in powers of ϵ, we get

$$z^2S' + 2z = \gamma(1 - e^{-\varepsilon S'}) - ^1/_2\gamma\varepsilon^2S''e^{-\varepsilon S'}. \quad (2.10)$$

In the derivation of (2.10) from (1.15) it was assumed that $z \gg 1$ and $\epsilon^2S'' \ll 1$. The terms $2z$

and $^1/_2 \gamma\epsilon^2 S''$ exp $(-\epsilon S'')$ can be determined by perturbation theory. Then, in the principal order in the small quantity $(\sqrt{\gamma/\epsilon})^{-1}$, Eq. (2.10) can be written conveniently in the standard form

$$x^2\varphi_0(x) = 1 - e^{-\varphi_0(x)}, \tag{2.11}$$

where

$$z = x\sqrt{\gamma\varepsilon}, \quad \varphi(x) = +\varepsilon S'(z). \tag{2.12}$$

Equation (2.11) defines an even function $\varphi(x)$ (we have discarded the trivial solution $\varphi = 0$). When x^2 is close to unity, φ is close to zero, and the solution of (2.11) can be written in the form

$$\varphi(x) \approx 2(1 - x^2). \tag{2.13}$$

For V(z) in the vicinity of the points $z = \pm z_0$ we obtain

$$V(z) = C\exp\left\{\sqrt{\frac{\gamma}{\varepsilon}}\int_{\pm 1}^{x}\varphi(x)\,dx\right\}$$

$$= C_1\exp\left\{2\sqrt{\frac{\gamma}{\varepsilon}}\left(x - \frac{x^3}{3}\right)\right\} = C_1 e^{\xi(z)}.$$

Thus, solutions of the type $Ae^{\xi(z)}$ are made continuous with the solutions of the type

$$V(z) = C\exp\left\{\sqrt{\frac{\gamma}{\varepsilon}}\int_{\pm 1}^{x}\varphi(x)\,dx\right\}. \tag{2.14}$$

Let us outline the region in which such solutions are defined. One limitation is imposed by the requirement

$$|\gamma\varepsilon^2 S'' e^{-\varepsilon S'}| \ll |\gamma(1 - e^{-\varepsilon S'}) - z^2 S'|,$$

which leads to the inequality

$$|z \pm z_0| \gg \gamma^{1/4}\varepsilon^{3/4}. \tag{2.15}$$

The other condition we already know: $|z| \gg 1$.

Let us determine the asymptotic behavior of $\varphi(x)$ when x is large. When $x^2 \gg 1$ we can neglect unity in the right side of (2.11) and obtain approximately

$$\varphi(x) \approx -\ln\{x^2|\ln x^2|\}.$$

Substituting the obtained asymptotic expression in (2.14) we find that solutions of this type increase exponentially as $z \to -\infty$. It follows therefore that the coefficient A_- in the solution (2.7) is equal to zero. Thus, the solution in the vicinity of the point $z = -z_0$ is defined, apart from the factor B_-.

Let us see what happens to the solution

$$e^{\xi(z)}\int_{-\infty}^{z} e^{-\xi(z)}dz$$

when $z - z_0 \gg \gamma^{1/4}\epsilon^{3/4}$. In this case we can neglect the term with the second derivative in (2.4) and obtain

$$V(z) = B_-/(z^2 - \gamma\varepsilon). \tag{2.16}$$

Comparing (2.16) with (1.17), we see that the coefficient B_- coincides with the sought number of levels N(E). The problem is now to express B_- in terms of the quantity A_+, which determines essentially the normalization of the function V(z).

We already know (see (2.8)) that V(z) in the region of $|z| \gg 1$, $|z + z_0| \gg \gamma^{1/4}\epsilon^{3/4}$ takes the form

$$V(z) = C_-\exp\left\{\sqrt{\frac{\gamma}{\varepsilon}}\int_{-1}^{x}\varphi(x)\,dx\right\},$$

$$C_- = 2\sqrt{\pi}\,B_-\gamma^{1/4}\varepsilon^{3/4}, \tag{2.17}$$

where $\varphi = \varphi_0 + \varphi_1$, $\varphi_0(x)$ is determined by Eq. (2.11), and φ_1 takes the form

$$\varphi_1(x) = -\sqrt{\frac{\varepsilon}{\gamma}}\,\frac{2x + {}^1/_2\varphi_0' e^{-\varphi_0}}{x^2 - e^{-\varphi_0}}. \tag{2.18}$$

We note that when $|x| \ll 1$ the term $\exp(-\varphi_0)$ in the right side of (2.11) is negligibly small. It is therefore natural to neglect the term $V(z - \epsilon)$ in the right side of (1.15) in the region $|x| \ll 1$, as will be justified. Solving the differential equation obtained in such an approximation, we get

$$V(z) = D\frac{e^{\gamma\tan^{-1}z}}{1 + z^2}. \tag{2.19}$$

In the region $1 \ll |z| \ll \sqrt{\gamma\epsilon}$ $(z < 0)$ this solution should go over into (2.17), for which purpose it is necessary to have

$$De^{-\gamma\pi/2} = C_-\exp\left\{\sqrt{\frac{\gamma}{\varepsilon}}\int_{-1}^{0}\left(\varphi(x) - \frac{1}{x^2} + 2\sqrt{\frac{\varepsilon}{\gamma}}\,\frac{1}{x}\right)dx\right\}. \tag{2.20}$$

The solution in the vicinity of $z \gg 1$, $z_0 - z \gg \gamma^{1/4}\epsilon^{3/4}$ goes over into a function of the type (2.17):

$$V(z) = C_+\exp\left\{\sqrt{\frac{\gamma}{\varepsilon}}\int_{1}^{x}\varphi(x)\,dx\right\}. \tag{2.21}$$

The connection between D and C_+ is similar to (2.20):

$$De^{1/2\gamma\pi} = C_+\exp\left\{\sqrt{\frac{\gamma}{\varepsilon}}\int_{1}^{0}\left(\varphi(x) - \frac{1}{x^2} - 2\sqrt{\frac{\varepsilon}{\gamma}}\,\frac{1}{x}\right)dx\right\} \tag{2.22}$$

(φ is defined as before). Finally, the solution (2.22) goes over into the solution (2.5), the connection between C_+ and A_+ being of the form

$$C_+\exp\left\{-\frac{4}{3}\sqrt{\gamma/\varepsilon}\right\} = A_+. \tag{2.23}$$

We are now in position to write an equation relating B_- with A_+:

$$B_- = (2\sqrt{\pi}\gamma^{1/4}\varepsilon^{3/4})^{-1}\exp\left\{-\gamma\pi - \sqrt{\frac{\gamma}{\varepsilon}}\int_{-1}^{1}\left(\varphi_0(x)-\frac{1}{x^2}\right)dx - \frac{4}{3}\sqrt{\frac{\gamma}{\varepsilon}}\right\}A_+. \quad (2.24)$$

Let us determine A_+ from the normalization condition

$$A_+ \approx \left[\int e^{\xi(z)}dz\right]^{-1} \approx \left[2\sqrt{\pi}\,\gamma^{1/4}\varepsilon^{3/4}\exp\left(\frac{4}{3}\sqrt{\frac{\gamma}{\varepsilon}}\right)\right]^{-1}. \quad (2.25)$$

Hence

$$N(k^2) \approx \frac{1}{2}k\gamma\varepsilon^2 B_- = \frac{1}{4\pi}\sqrt{\frac{a}{\bar{l}}}\exp\left\{-\frac{\pi}{k\bar{l}} + \frac{1}{\sqrt{a\bar{l}}}\int_{-1}^{+1}\left(\frac{1}{x^2}-\varphi_0(x)\right)dx\right\}. \quad (2.26)$$

In the course of the work we had to introduce one more limitation $\epsilon \ll \gamma$ (see (2.10), (2.11), and (2.18)). However, this limitation is not essential. It can be readily lifted by replacing the function $\varphi_0(x)$ in the integral (2.26) by means of a more complicated function, calculated with the aid of the ordinary differential equation

$$x^2\varphi + 2\sqrt{\varepsilon/\gamma}\,x = 1 - e^{-\varphi}(1 + {}^1/_2\sqrt{\varepsilon/\gamma}\,\varphi').$$

N(E), and consequently also dN/dE, is proportional to the exponential $\exp(-\pi/k\bar{l})$. This result can be readily interpreted from the physical point of view. When the particle has a wavelength λ much larger than the average distance between neighboring centers $\bar{l}$, its average energy becomes of the order of $a/\bar{l}$. The energy $k^2 \ll a/\bar{l}$ $(\epsilon\gamma \gg 1)$ can be obtained only in those configurations or on that section of the chain, where the neighboring lattice points have been moved apart by a distance of the order of $\pi/2$, in order to make room for at least one node of the wave function. Since the probability is $P(l) = \bar{l}^{-1}\exp(-l/\bar{l})$, the statistical weight of such states should be proportional to $\exp(-\lambda/2\bar{l}) = \exp(-\pi/kl)$. Of course, the factor π in the exponent follows from our non-rigorous considerations.

This reasoning can be made more precise by taking into account the finite height of the well walls.[2)] Then the electron wave function is not localized exactly in the well, but "seeps in" to a depth

$$\delta \sim \left\{\frac{1}{\bar{l}}\int_0^{\bar{l}} V(x)\,dx\right\}^{-1/2} \sim \left(\frac{a}{\bar{l}}\right)^{-1/2}.$$

Thus, in order for the low-probability state with $\lambda \gg \bar{l}$ to be produced, it is necessary that the neighboring lattice points move apart a distance $\sim \lambda/2 - 2\delta$. The probability of such a fluctuation is of the order of

$$\exp\left\{-\frac{\lambda}{2\bar{l}} + \frac{2\delta}{\bar{l}}\right\} = \exp\left\{-\frac{\pi}{k\bar{l}} + \frac{2}{\sqrt{a\bar{l}}}\right\}, \quad (2.27)$$

in accord with (2.26). In the derivation of (2.27) it is implied, of course, that $\delta \gg \bar{l}$. This is equivalent to the inequality $\gamma \gg \epsilon$ used in the derivation (2.26). The coefficient preceding the term $\delta/\bar{l}$ (which is of the order of unity) is connected with a certain effective smearing of the edges of the well, which depends essentially on the form of the distribution of the distances between the lattice points and, of course, cannot be established from reasoning of this kind.

3. CORRELATION FUNCTION OF THE NEIGHBORING POINTS P(l) ARBITRARY

We assume as before that $E \ll \overline{V}$ $(\epsilon\gamma \gg 1)$. A solution of the general equation (1.2) for the case when P(l) with l large decreases more rapidly than an arbitrary power l^{-n} can be obtained in similar fashion. In the regions $|z^2 - z_0^2| \ll \gamma\epsilon$ the function V(z') in the integral can be expanded in powers of the difference $z' - z$. The resultant differential equation differs from (2.4) in an additional factor α preceding V''(z), where

$$\alpha = (\bar{l}^2 - \bar{l}^2)/\bar{l}^2. \quad (3.1)$$

Without repeating the reasoning of Sec. 2, we write out the solution V(z) in the vicinity of the point $-z_0$ in the form

$$V(z) = B_- e^{\xi(z)/\alpha}\int_{-\infty}^{z} e^{-\xi(z)/\alpha}\,dz. \quad (3.2)$$

A good approximation for V(z) in the region $|z + z_0| \gg \gamma^{1/4}\epsilon^{3/4}$, $z \gg 1$

$$V(z) = C_-\exp\left\{\sqrt{\frac{\gamma}{\varepsilon}}\int_{-1}^{x}\varphi(x)\,dx\right\},\quad C_- = 2B_-\sqrt{\alpha\pi}\,\gamma^{1/4}\varepsilon^{3/4}, \quad (3.3)$$

where $\varphi(x)$ satisfies the equation

$$\varphi = \varphi_0 + \varphi_1,\quad e^{\varphi_0} = \hat{P}(-\varphi_0 x^2),$$

$$\varphi_1 = \sqrt{\frac{\varepsilon}{\gamma}}[x^2\hat{P}'(-\varphi_0x^2) - \hat{P}(-\varphi_0x^2)]^{-1}\left\{x\hat{P}'(-\varphi_0x^2) + \frac{1}{2}\frac{d\varphi_0}{dx}[\hat{P}(-\varphi_0x^2) - 2x^2\hat{P}'(-\varphi_0x^2) + x^4\hat{P}''(-\varphi_0x^2)]\right\};$$

$$\hat{P}(\nu) = \int e^{-\nu l/\bar{l}}P(l)\,dl,\quad \hat{P}'(\nu) = \frac{d\hat{P}(\nu)}{d\nu}. \quad (3.4)$$

[2)] The authors are indebted to Yu. A. Bychkov and A. N. Dykhne for this remark.

In the region $x \ll 1$, it is more convenient to deal with $W(\psi)$ and to use the initial equation (1.10). The main contribution to the integral is made by the region of the maximum $|\psi - \psi_0| \sim \epsilon^{-1/4}\gamma^{-3/4}$. The connection between ψ, ψ', and l for small ψ' can be approximately written in the form

$$\psi' = \psi + k(\bar{l} - l).$$

This means that the equality $kl \approx \psi$ is satisfied in the essential region of integration in (1.10). Assuming that for large $l \gg \bar{l}$ the distribution $P(l)$ has an asymptotic form $P(l) \sim \exp(-\tilde{\gamma} k l)$, we obtain in the region $x \ll 1$ a solution in the form

$$W(\psi) = De^{-\tilde{\gamma}\psi}. \tag{3.5}$$

Joining together (3.5) with (3.3), we obtain

$$e^{-\tilde{\gamma}\pi}D = C\exp\left\{\sqrt{\gamma}\int_{\varepsilon-1}^{0}\left(\varphi(x) - \frac{\tilde{\gamma}}{\gamma}\frac{1}{x^2}\right)dx + \frac{\tilde{\gamma}}{\sqrt{\gamma\varepsilon}}\right\}.$$

In similar fashion we continue the joining together and find ultimately

$$N(k^2) = \frac{1}{4\pi}\sqrt{\frac{a}{\bar{l}}}\exp\left\{-\pi\tilde{\gamma} + \frac{1}{\sqrt{a\bar{l}}}\int_{-1}^{1}\left(\frac{\tilde{\gamma}}{\gamma x^2} - \varphi_0(x)\right)dx\right\}. \tag{3.6}$$

It is obvious that the physical meaning of the result is the same as in the preceding section.

It should be noted that if the impurities are close to one another, then interaction sets in between them and a deviation from the Poisson law appears when $l < \bar{l}$. Thus, the interaction of the impurities at large distances influences the form of $\varphi_0(x)$ and has a substantial effect on the second term in the exponential in (3.6).

We see that the structure of the edge of the band is determined by the asymptotic behavior of $P(l)$ for large $l \gg \lambda$. In particular, for a Gaussian distribution the level density at the bottom of the band has an entirely different form, viz., $N(E) \sim \exp(-A/k^2)$, where A is a constant. Thus, there is no universal answer to our question. To the contrary, knowing the density of the levels at the edge of the band, we can judge the character of the distribution function of the distances between lattice points.

We are grateful to A. Z. Patashinskiĭ for a useful discussion.

APPENDIX 1

The motion of an electron in a random field V(x) is treated in a number of papers (see, for example, [7,8]). We assume for the field V(x) a Gaussian distribution

$$\langle V(x)\rangle = 0, \quad \langle V(x)V(x')\rangle = V_0^2\delta(x - x'). \tag{A1.1}$$

We shall show that the method developed in this paper leads directly to the solution of the problem with the spectrum of the electron in the field (A1.1).

Assume that the coefficient a in (1.1) depends on the number i and can assume two values $\pm a$ ($a > 0$), each with probability $1/2$. Then we get in place of (1.10)

$$W(\psi) = \frac{1}{2}\int dlP(l)\left\{W(\psi'(\psi,l))\frac{d\psi'(\psi,l)}{d\psi} + W(\psi''(\psi,l))\frac{d\psi''(\psi,l)}{d\psi}\right\}, \tag{A1.2}$$

where

$$\operatorname{ctg}\psi' = \operatorname{ctg}(\psi - l) - \varepsilon, \quad \operatorname{ctg}\psi'' = \operatorname{ctg}(\psi - l) + \varepsilon. \tag{A1.3}$$

In analogy with the derivation of (1.15), we get

$$\frac{1}{\gamma}\frac{d}{dz}[(1+z^2)V(z)] = V(z) - \frac{1}{2}\{V(z-\varepsilon) + V(z+\varepsilon)\}. \tag{A1.4}$$

If we now take the limit as

$$\varepsilon \to 0, \quad \gamma \to \infty, \quad \varepsilon^2\gamma = \text{const} = {}^1/_2V_0^2, \tag{A1.5}$$

then the distribution of the value V(x) goes over into the Gaussian distribution (A1.1).[9] Expanding now $V(z \pm \epsilon)$ in (A1.4) in powers of ϵ and making the transition (A1.5), we obtain

$$\frac{d}{dz}[(1+z^2)V(z)] + \frac{1}{2}V_0^2\frac{d^2V}{dz^2} = 0. \tag{A1.6}$$

Equation (1.19) for the number of states N(E) takes in this case the form

$$N(E) = \frac{1}{\pi} + \frac{\gamma}{\pi}\int_{-\infty}^{\infty}\operatorname{arcctg} z\left\{\frac{1}{2}V(z-\varepsilon) + \frac{1}{2}V(z+\varepsilon) - V(z)\right\}dz. \tag{A1.7}$$

Substitution of (A1.4) in (A1.7) leads to

$$N(E) = \lim_{z\to-\infty} z^2V(z).$$

Equation (A1.6) for V(z) can be easily solved, and the number of states N(E) can be expressed in terms of Airy functions.[10]

APPENDIX 2

Assume that we are given

$$P(l) = \gamma^2 l e^{-\gamma l}, \quad \int_0^\infty P(l)\,dl = 1, \quad \bar{l} = \frac{2}{\gamma}. \tag{A2.1}$$

By differentiating (1.10) twice with respect to ψ we obtain, in analogy with the derivation of (1.15)

$$\frac{d}{dz}\left\{(1+z^2)\frac{d}{dz}[(1+z^2)V(z)]\right\}$$
$$=2\gamma\frac{d}{dz}[(1+z^2)V(z)]+\gamma^2[V(z-\varepsilon)-V(z)]. \quad \text{(A2.2)}$$

Substitution of (A2.2) in (1.19) yields

$$N(E)=\lim_{z\to-\infty}\left\{z^2V(z)-\frac{1}{2\gamma}z^2\frac{d}{dz}(z^2V)\right\}. \quad \text{(A2.3)}$$

The result shows that formula (1.17) is not universal.

[1] F. J. Dyson, Phys. Rev. **92**, 1339 (1953).
[2] I. M. Lifshitz, UFN **83**, 617 (1964), Soviet Phys. Uspekhi **7**, 549 (1965).
[3] E. W. Montroll and R. B. Potts, Phys. Rev. **102**, 72 (1956).
[4] H. Schmidt, Phys. Rev. **105**, 425 (1957).
[5] H. L. Frish and S. P. Lloyd, Phys. Rev. **120**, 1175 (1960).
[6] S. O. Rice, Bell System Tech. J. **23**, 282 (1944).
[7] S. F. Edwards, Proc. Phys. Soc. **85**, Part 1, 543 (1965).
[8] I. V. Andreev, JETP **48**, 1437 (1965), Soviet Phys. JETP **21**, 961 (1965).
[9] M. A. Leibowitz, J. Math, Phys. **4**, 852 (1963).
[10] B. I. Halperin, Phys. Rev. **139**, 104A (1965).

Translated by J. G. Adashko
52