IMPURITY BAND IN A ONE-DIMENSIONAL MODEL

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We have found the electron energy level density in the neighborhood of an impurity level when the impurities are randomly distributed. We consider a one-dimensional model where one can solve the problem exactly. The impurity band found turns out to be asymmetric and to have an asymmetric singularity.

THE present paper is devoted to finding the electron energy spectrum in the neighborhood of an impurity level corresponding to one isolated center. We consider a one-dimensional model for which the problem has an exact solution. The electron moves in the field of randomly distributed attractive δ-function-like centers for which we shall assume a Poisson distribution.

Frish and Lloyd[1] have shown that finding the spectrum reduces to solving the equation

$$\frac{d}{dz}[(z^2-k^2)f(z)]+\frac{1}{a}[f(z+2k_0)-f(z)]=0. \quad (1)$$

Here $k^2 = -2mE$ ($E < 0$), $k_0^2 = 2m|E_0|$ ($k_0 > 0$), E_0 is the level corresponding to one center, a the average distance between the centers. The integral level density $N(E)$ can be found from the relation

$$\frac{N(E)}{L}=\lim_{z\to\infty} z^2 f(z). \quad (2)$$

Here $f(z)$ is the solution of Eq. (1) which satisfies the normalization condition

$$\int_{-\infty}^{\infty} f(z)\,dz=1. \quad (3)$$

We introduce the Fourier transform

$$g(t)=\int_{-\infty}^{\infty} f(z)e^{itz}\,dz.$$

To find the equation satisfied by $g(t)$ we multiply (1) by e^{itz} and integrate over z. We have:

$$\int_{-\infty}^{\infty} e^{itz}\frac{d}{dz}[(z^2-k^2)f(z)]\,dz+\frac{1}{a}(e^{-2ik_0t}-1)g(t)=0. \quad (4)$$

When $t \neq 0$ we can in (4) integrate by parts and we must then assume that $t\,\mathrm{Im}\,z > 0$. The function $g(t)$ will satisfy the equation

$$g''(t)+k^2g(t)+\frac{e^{-2ik_0t}-1}{ita}g(t)=0. \quad (5)$$

It follows from the derivation that the solution which we are looking for which decreases as $t \to \pm\infty$ consists, in general, of two different analytical functions for $t > 0$ and $t < 0$. From the normalization condition (3) follows that

$$g(0)=1. \quad (6)$$

The inverse transformation has the form

$$f(z)=\frac{1}{2\pi}\int_{-\infty}^{\infty} g(t)e^{-itz}\,dt. \quad (7)$$

Twice integrating by parts in (7) we find

$$f(z)=-\frac{1}{2\pi z^2}\int_{-\infty}^{\infty} g''(t)e^{-itz}\,dt. \quad (8)$$

Using (2) we find

$$\frac{N(E)}{L}=-\frac{1}{2\pi}\lim_{z\to\infty}\int_{-\infty}^{\infty} e^{-itz}g''(t)\,dt, \quad (9)$$

whence

$$\frac{N(E)}{L}=\frac{1}{2\pi}[g'(-0)-g'(+0)]. \quad (10)$$

We introduce the dimensionless variable $\tau = kt$. We get

$$g''(\tau)+\omega^2(\tau)g(\tau)=0, \quad (11)$$

where

$$\alpha=\frac{1}{ka},\quad \gamma=k_0/k,\quad \omega^2(\tau)=1+\frac{\alpha}{i\tau}(e^{-2i\gamma\tau}-1). \quad (12)$$

Condition (10) becomes

$$\frac{N(E)}{L}=\frac{k}{2\pi}[g'(-0)-g'(+0)]. \quad (13)$$

We note that if $g(\tau)$ is a solution of Eq. (11) for real τ, then $g^*(-\tau)$ is also a solution. Using this fact, we transform (13) to the final form

$$\frac{N(E)}{L}=-\frac{k}{\pi}\,\mathrm{Re}\,g'(+0). \quad (14)$$

To find the level density we must thus find the solution of Eq. (11) which decreases as $\tau \to +\infty$

and which satisfies Eq. (6). The value of the derivative $g'(\tau)$ at zero is connected with the level density through Eq. (14).

We shall consider an "impurity band," which means that each impurity attracts an electron ($k_0 > 0$). The impurity density is small ($\alpha \ll 1$). Finally, we are interested in energies close to the level of an isolated impurity ($k \approx k_0$). The presence of small parameters, $\alpha \ll 1$ and $\kappa = 1 - \gamma \ll 1$, appreciably simplifies the study of Eq. (11).

Let us qualitatively explain the situation arising when we solve Eq. (11). The small (of order α) increment to unity in Eq. (12) can not be taken into account by perturbation theory, since it decreases slowly ($\sim 1/\tau$) for large τ. Moreover, when $\kappa \ll 1$ the presence of the factor $e^{-2i\gamma\tau}$ leads to a peculiar parametric resonance, somewhat reduced by the presence of the factor $1/\tau$. Formally, Eq. (11) satisfies the condition for semi-classical behavior $d\omega/d\tau \sim \alpha \ll 1$. However, applying the standard procedure connected with going round the complex "turning" points does in this case not lead to the goal, as it is shown by analysis that there are many such points and that they must be taken into account simultaneously.

We shall look for a solution in the form

$$g(\tau) = A(\tau)\frac{1}{\sqrt{\omega}}\exp\left(i\int_0^\tau \omega d\tau'\right) + B(\tau)\frac{1}{\sqrt{\omega}}\exp\left(-i\int_0^\tau \omega d\tau'\right), \tag{15}$$

where $A(\tau)$ and $B(\tau)$ are two new unknown functions. Imposing upon then the additional condition

$$g'(\tau) = \frac{i\omega}{\sqrt{\omega}}\left[A(\tau)\exp\left(i\int_0^\tau \omega d\tau'\right) - B(\tau) \times \exp\left(-i\int_0^\tau \omega d\tau'\right)\right], \tag{16}$$

we get for A and B a set of equations:

$$A'(\tau) = \frac{\omega'}{2\omega}\exp\left(-2i\int_0^\tau \omega d\tau'\right)B(\tau),$$

$$B'(\tau) = \frac{\omega'}{2\omega}\exp\left(2i\int_0^\tau \omega d\tau'\right)A(\tau). \tag{17}$$

The right-hand sides of Eqs. (17) are small ($\sim\alpha$) so that A and B change slowly. To find the boundary conditions which A and B must satisfy as $\tau \to \infty$, we note that for large τ

$$\exp\left(\pm i\int_0 \omega d\tau'\right) \to \tau^{\mp\alpha/2}\exp(\pm i\tau). \tag{18}$$

It is clear from this that for $g(\tau)$ to decrease we must put $B(\infty) = 0$.

We shall solve the set (17) by iteration. As we shall show in Appendix 1, it is then sufficient to restrict ourselves to the zeroth approximation for A ($A_0 \equiv A(\infty)$) and the first one for B. We have

$$B(\tau) = -A_0\int_\tau^\infty \frac{\omega'}{2\omega}\exp\left(2i\int_0^\tau \omega d\tau'\right)d\tau.$$

It is clear from (15) and (16) that to find the level density it is sufficient to know $B(0)$:

$$\frac{B(0)}{A_0} = -\int_0^\infty \frac{\omega'}{2\omega}\exp\left(2i\int_0^\tau \omega d\tau'\right)d\tau. \tag{19}$$

Integrating in (19) by parts we find

$$B(0) = \alpha\gamma A_0 + A_0 i\int_0^\infty \omega\ln\omega\exp\left(2i\int_0^\tau \omega d\tau'\right)d\tau. \tag{20}$$

Taking it into account that $|\omega - 1| \ll 1$, we find

$$B(0) = \frac{\alpha A_0}{2}\int_0^\infty \frac{e^{-2i\gamma\tau}-1}{\tau}\exp\left(2i\int_0^\tau \omega d\tau'\right)d\tau. \tag{21}$$

For what follows it is convenient to transform the expression

$$2i\int_0^\tau \omega d\tau$$

$$\approx 2i\tau + \alpha\int_0^\tau \frac{\cos 2\gamma\tau - 1}{\tau}d\tau - i\alpha\int_0^\tau \frac{\sin 2\gamma\tau}{\tau}d\tau$$

$$= 2i\tau - \frac{i\alpha\pi}{2} - \alpha\ln\tau + i\alpha\int_\tau^\infty \frac{\sin 2\gamma\tau}{\tau}d\tau$$

$$+ \alpha\int_0^1 \frac{\cos 2\gamma\tau - 1}{\tau}d\tau + \alpha\int_1^\tau \frac{\cos 2\gamma\tau}{\tau}d\tau.$$

Large τ give the main contribution to the integral over τ in (21). Then, with the required accuracy,

$$\exp\left(2i\int_0^\tau \omega d\tau'\right) \approx 1 - \frac{i\alpha\pi}{2}\quad \tau^{-\alpha}\exp(2i\tau), \tag{22}$$

$$B(0) = \frac{A_0\alpha}{2}\left(1 - \frac{i\alpha\pi}{2}\right)I, \tag{23}$$

where

$$I = \int_0^\infty \frac{e^{2i\varkappa\tau} - e^{2i\tau}}{\tau^{1+\alpha}}d\tau. \tag{24}$$

Calculation of I, which is done in Appendix 2, leads to the result

$$I = \frac{1}{\alpha}(1 - |\varkappa|^\alpha) + \frac{i\pi}{2}\left(\frac{\varkappa}{|\varkappa|}|\varkappa|^\alpha - 1\right). \tag{25}$$

Substituting (25) into (23) and using Eq. (6), as well as (14) and (16), we get an expression for the integral density:

$$\frac{N(E)}{\mathfrak{N}} = 4\frac{1-|\varkappa|^{\alpha}\theta(\varkappa)}{(3-|\varkappa|^{\alpha})^2}, \quad \theta(x) = \begin{cases} 1, & x>0 \\ 0, & x<0 \end{cases}, \quad (26)$$

where $\mathfrak{N}$ is the number of impurities.

Expressing $\kappa = 1 - k_0/k$ in terms of $\epsilon = (E - E_0)/|E_0|$ we get finally

$$\frac{N(E)}{\mathfrak{N}} = 4\frac{1-|\varepsilon|^{\alpha}\theta(-\varepsilon)}{(3-|\varepsilon|^{\alpha})^2} + O(\alpha, \varepsilon). \quad (27)$$

We give the expression for the spectral density

$$\rho(\varepsilon) = \mathfrak{N}^{-1} dN(\varepsilon)/d\varepsilon:$$

$$\rho(\varepsilon) = \begin{cases} \dfrac{8\alpha|\varepsilon|^{\alpha-1}}{(3-|\varepsilon|^{\alpha})^3}, & \varepsilon>0 \\ \dfrac{4\alpha|\varepsilon|^{\alpha-1}(1+|\varepsilon|^{\alpha})}{(3-|\varepsilon|^{\alpha})^3}, & \varepsilon<0 \end{cases} \quad (28)$$

The formulae found here solve completely the problem of studying the spectrum of the impurity band in the chosen model. It follows from the derivation that Eq. (27) is valid for small α and $|\epsilon|$ but for arbitrary ratios of these two quantities.

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It is clear from (27) that the only parameter determining the result is $\alpha \ln|\epsilon|$. We see then:

1. The quantity

$$\frac{N(\varepsilon)}{\mathfrak{N}} \to \begin{cases} 0, & \varepsilon<0 \\ 1, & \varepsilon>0 \end{cases} \text{when } \alpha\ln|\varepsilon| \ll 1. \quad (29)$$

The impurity band contains thus in the approximation considered $\mathfrak{N}$ levels, i.e., there is no overlap with the continuous spectrum.

2. As $\epsilon \to 0$, $\alpha \ln|\epsilon| \gg 1$ and it follows from (28) that the spectral density has the form

$$\rho(\varepsilon) = \begin{cases} \dfrac{8}{27}\alpha|\varepsilon|^{\alpha-1}, & \varepsilon>0 \\ \dfrac{4}{27}\alpha|\varepsilon|^{\alpha-1}, & \varepsilon<0 \end{cases}.$$

The spectral density has thus an integrable singularity at $\epsilon = 0$ and the main term turns out to be asymmetric with respect to the point $\epsilon = 0$.

3. For ϵ which are sufficiently large (but small compared to unity) the integral density has the form

$$\rho(\varepsilon) = \alpha|\varepsilon|^{-1}, \quad \alpha\ln|\varepsilon| \ll 1 \quad (31)$$

and turns out to be symmetric with respect to $\epsilon = 0$.

4. As a measure of the asymmetry of the impurity band we can use the number of levels less than E_0:

$$N(0)/\mathfrak{N} = 4/9. \quad (32)$$

We note that I. M. Lifshitz had considered this problem approximately.[2] The approach given in[2] can equally well be applied to three- and one-dimensional problems. Comparison shows that the results obtained in[2] are only qualitatively correct. In fact, only the singularity in the spectrum $\rho(\epsilon) \propto |\epsilon|^{\alpha-1}$ was found correctly. The coefficients were not found in that approximate treatment.

APPENDIX 1

We shall show that the corrections to solution (18) of the set (17) are small. We restrict ourselves to considering the second iteration for A. Estimates of the other iterations can be made similarly and do not cause any difficulties. Substituting (18) into (17) we find

$$\frac{A(\tau)}{A(\infty)} = 1 + \frac{1}{4}\int_{\tau}^{\infty} \frac{\omega'(\tau_1)\,d\tau_1}{\omega(\tau_1)} \exp\left(-2i\int_0^{\tau_1}\omega\,d\tau_2\right)$$
$$\times \int_{\tau_1}^{\infty} \frac{\omega'(\tau_3)}{\omega(\tau_3)} \exp\left(2i\int_0^{\tau_3}\omega d\tau_4\right) d\tau_3. \quad (1.1)$$

The correction to unity in (1.1) is proportional to α. Any complications are only to be expected for large values of the integration variables in (1.1). We have

$$\frac{A(0)}{A(\infty)} = 1 - \alpha^2\int_0^{\infty} \frac{e^{-2i\gamma\tau}-1}{\tau} \exp\left(-2i\int_0^{\tau}\omega\,d\tau'\right) d\tau$$
$$\times \int_{\tau}^{\infty} \frac{e^{-2i\gamma\tau_1}-1}{\tau_1} \exp\left(2i\int_0^{\tau_1}\omega\,d\tau'\right) d\tau_1 + O(\alpha^2). \quad (1.2)$$

When changing from (1.1) to (1.2) we have integrated by parts, and the terms outside the integral are small. We show that the integral in (1.2) is bounded. The interior integral contains "dangerous" terms of two kinds: $1/\alpha\tau^{\alpha}$ and $e^{2i\tau}/\tau^{1+\alpha}$ (we use the asymptotic value of (18)). When substituting terms of the first type into (1.2) we get

$$\frac{A(0)}{A(\infty)} - 1 \sim \alpha\int_0^{\infty} \frac{e^{-2i\tau}-e^{4i\tau}}{\tau}\,d\tau + O(\alpha^2).$$

This expression is $\sim\alpha^2$ (convergence is attained because of oscillations). When substituting terms of the second type we have

$$\frac{A(0)}{A(\infty)} - 1 \sim \alpha^2\int_1^{\infty} \frac{d\tau}{\tau^2} + O(\alpha^2).$$

The general situation arising when estimating terms of arbitrary order can be reduced to one or the two variants considered. A large result can be obtained only when there are present resonance (non-oscillating) integrands which at the same time decrease slowly ($\sim 1/\tau^{1+\alpha}$) at infinity. However, as in the example considered above, at least one of these conditions is violated in all approximations, except the first one for B, which is considered in the text and in Appendix 2.

APPENDIX 2

Separating in (24) the real and imaginary parts ($I = I' + iI''$) we get

$$I' = \int_0^\infty \frac{\cos 2\varkappa\tau - 1}{\tau^{1+\alpha}} d\tau - \int_0^\infty \frac{\cos 2\tau - 1}{\tau^{1+\alpha}} d\tau, \quad (2.1)$$

$$I'' = \int_0^\infty \frac{\sin 2\varkappa\tau}{\tau^{1+\alpha}} d\tau - \int_0^\infty \frac{\sin 2\tau}{\tau^{1+\alpha}} d\tau. \quad (2.2)$$

In the first of the integrals in (2.2) we make the substitution $\xi = |\kappa|\tau$, which leads to the following result:

$$I'' = \left(\frac{\varkappa}{|\varkappa|} |\varkappa|^\alpha - 1\right) \int_0^\infty \frac{\sin 2\xi}{\xi^{1+\alpha}} d\xi. \quad (2.3)$$

The integral occurring in (2.3) is regular in α for small α. For the main order we have

$$I'' = \frac{\pi}{2}\left(\frac{\varkappa}{|\varkappa|} |\varkappa|^\alpha - 1\right). \quad (2.4)$$

A similar substitution applied to I' leads to the result

$$I' = (|\varkappa|^\alpha - 1) \int_0^\infty \frac{\cos 2\tau - 1}{\tau^{1+\alpha}} d\tau. \quad (2.5)$$

In the main order in α we have, as can be checked easily,

$$\int_0^\infty d\tau \frac{\cos 2\tau - 1}{\tau^{1+\alpha}} = \frac{1}{\alpha} + O(1). \quad (2.6)$$

From (2.4) to (2.6), (25) follows:

[1] H. L. Frish and S. P. Lloyd, Phys. Rev. **120**, 1175 (1960).

[2] I. M. Lifshitz, JETP **44**, 1723 (1963), Soviet Phys. JETP **17**, 1159 (1963).

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