Energy level correlations in a disordered one-dimensional chain

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The spatial dependence of the density-of-states correlator for energetically close states in a linear chain containing defects is found. The curve obtained can be interpreted as indicating the existence of attraction between close states over distances of the order of the mean free path l. Next, there is a dip—an interlevel repulsion region extending to distances of the order of $z_0 = 2l \ln(8/\nu)$ (where ν is a dimensionless energy difference). The pattern of independent levels is restored at large distances. It is shown that in the case of a finite chain of great length (greater than z_0) the levels of the system as a whole are statistically independent.

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1. INTRODUCTION

Back in 1961 Mott and Twose[1] adduced convincing arguments to show that, in a one-dimensional system, the electron wave functions for all energies are localized in the presence of impurities or defects. A mathematically rigorous proof of this fact was given by Berezinskiĭ,[2] who, in particular, found a frequency dependence of the conductivity, that basically agrees with the predictions made in Ref. 1.

The concept of centers on which the electron is localized in the first approximation is used in the argumentation in Ref. 1. The tunneling overlap of wave functions on different centers splits the levels of the centers, and guarantees transitions between them. In applications (to quasi-one-dimensional organic metals, for example), the first approximation corresponds rather to a one-dimensional metallic band, and the localization is a result of the quantum interference effects due to the multiple scattering on the impurities.[2] The electron wave functions (at least in the quasiclassical region, which will be discussed below) oscillate rapidly over atomic distances, i.e., over distances $\sim\hbar/p_F$, and only their envelopes decay over distances of the order of the localization length, which is of the order of the mean free path.[2,3]

Thus, contrary to the relatively simple picture painted in Ref. 1, the exact electron wave functions are a rather complicated object, and in Refs. 2 and 3 quite a complicated diagrammatic technique is used to compute the corresponding averages from them. That simplifications connected with the specific nature of the one-dimensional problem are possible had been pointed out earlier by Schmidt[4] (see also Halperin's paper[5]). Subsequently, Schmidt's method[4] was successfully applied in Ref. 6 to the problem of computing density of states. Finally, in Ref. 7 a method is developed which allows us, at least in principle, to compute mean values of entirely general form, from an arbitrary combination of the exact wave functions of an electron localized in the field of defects.

The purpose of the present paper is to determine more accurately the scope of the ideas about electron localization, or, more strictly speaking, to determine the correlations between levels corresponding to close energy values. The greater part of the paper is devoted to the computation of the correlator for densities of states at different points:

$$F_{E,E+\omega}(x-x') = \left\langle \sum_{\rho\eta} \delta(E-\varepsilon_\rho)\,\delta(E+\omega-\varepsilon_\eta)\,\psi_\rho^2(x)\,\psi_\eta^2(x') \right\rangle, \tag{1}$$

where $\varepsilon_\rho, \varepsilon_\eta$ and ψ_ρ, ψ_η are respectively the exact energy levels and exact wave functions of states localized in the field of the defects and the brackets denote averaging over the disposition of the defects.

The correlator in (1) is defined for an arbitrary segment of an infinitely long chain. For a finite segment we can formulate a different problem concerning the correlation and repulsion of the exact energy levels of the whole system of fixed dimension L. The solution to the last problem is known,[8,9] and the answer is that there are no correlations. We shall briefly discuss this question in the last section.

2. THE DENSITY-OF-STATES CORRELATOR

The method developed in Ref. 7 is used below to compute (1). Let us, following (7), write the wave function of, say, the state ε_η in the form

$$\psi_\eta(x) = R_\eta(x)\,\sin\varphi_\eta(x). \tag{2}$$

The main variation of the phase in (2) (the rapid oscillations) is connected with the free motion: $\nabla\varphi \approx p_F$. At distances large compared to the atomic distances, the square of the wave function should be averaged in order to obtain a smoothed out density of states at the point x', i.e., we should make the substitution

$$\psi_\eta^2(x') \to {}^1/_2 R_\eta^2(x') \tag{3}$$

and similarly for $\psi_\rho(x)$. Therefore, for $|x-x'| \gg 1/p_F$, we shall everywhere replace (1) by

$$F_\omega(x-x') \equiv F_{E,E+\omega}(x-x') = \frac{1}{4}\left\langle \sum_{\rho\eta} \delta(E-\varepsilon_\rho)\,\delta(E+\omega-\varepsilon_\eta)\,R_\rho^2(x)\,R_\eta^2(x') \right\rangle. \tag{1'}$$

In the case of identically coincident x and x' the phases of the wave functions cannot be averaged independently:

$$F_\omega(x=x') = \frac{1}{4}\left\langle \sum_{\rho\eta} \delta(E-\varepsilon_\rho)\,\delta(E+\omega-\varepsilon_\eta)\,R_\rho^2(x)\,R_\eta^2(x')\left(\frac{1}{2}+\cos^2\theta_\omega\right) \right\rangle. \tag{4}$$

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Here

$$\theta_\omega = \varphi_\eta - \varphi_\rho \tag{5}$$

is the phase difference for the two states, which, generally speaking, changes over distances greater than, or of the order of, the mean free path, and carries the main information about the correlation of the states.

According to (7), if the potential of the defects has a sufficiently short range, then the problem of averaging expressions of the type (1), (1') reduces to Markov processes. For $x < x'$, it is convenient to take the point x' to be a matching point, and perform two independent averagings: one over the defects located to the right, the other over the defects located to the left, of x'. With (1) expressed in terms of the notation used in (7), let us, by transforming the energy δ function, rewrite it in the form

$$F_\omega(x-x') = \frac{1}{v_F^2}\int_0^\pi\int_0^\pi \langle \delta(\varphi_E^{>}(x') - \varphi_1)\,\delta(\varphi_{E+\omega}^{>}(x') - \varphi_2)$$

$$\times \delta(\varphi_1 - \varphi_E^{<}(x'))\,\delta(\varphi_2 - \varphi_{E+\omega}^{<}(x'))\,\alpha_E^2(x|x')\rangle\, d\varphi_1\, d\varphi_2,$$

where $\alpha(x|x') = R(x)/R(x')$.

For $p_F l \gg 1$, only the dependence on the relative phase difference (5) is important in the last expression, since the energy ε_ρ itself is not distinguished by anything in the quasiclassical limit. The steady-state probability distribution $w(\varphi,\theta)$ for the phases $\varphi \equiv \varphi_\rho$ and $\theta = \varphi_\eta - \varphi_\rho$ depends only on the phase difference θ:

$$w(\varphi, \theta) = w(\theta), \tag{6}$$

where the function $w(\theta)$ is found in Ref. 7. Finally, let us rewrite (1') in the form

$$F_\omega(x-x') = \frac{\pi}{v_F^2}\int_0^\pi g(x-x', \theta)\, w(\pi-\theta)\, d\theta, \tag{7}$$

where the equation for the function

$$g(x-x', \theta) = \langle \delta(\theta_\omega^{>}(x') - \theta)\,\alpha^2(x|x')\rangle \tag{8}$$

can easily be derived in accordance with Ref. 7:

$$\frac{\partial g}{\partial z} = \frac{\partial}{\partial\theta}\left(\sin^2\theta\,\frac{\partial g}{\partial\theta}\right) - \nu\frac{\partial g}{\partial\theta}. \tag{9}$$

Everywhere below we use the dimensionless notation

$$\nu = \omega\tau, \quad z = (x-x')/l, \quad x \to x/l,$$

where the quantities $l = v_F\tau$ and τ are the corresponding kinetic quantities–the mean free path and mean free time.

The boundary condition for (9) at $x = x'$ follows from the definition

$$g_\omega(x=x', \theta) = w(\theta). \tag{9'}$$

For coincident pints $x \equiv x'$ the expression (4) has the form

$$F_\omega(x\equiv x') = \frac{\pi}{v_F^2}\int_0^\pi w(\theta)\, w(-\theta)\left(\frac{1}{2} + \cos^2\theta\right) d\theta, \tag{4'}$$

and can be determined directly.

Before proceeding to carry out the computations, let us say something about Fig. 1, which schematically shows the

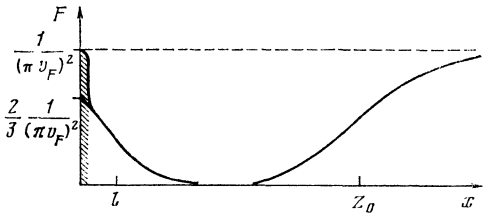

FIG. 1. Diagrammatic representation of the spatial dependence of the density-of-states correlator (1) for energetically close states. The region $z \sim l$ corresponds to the overlap of the corresponding wave functions. The hatched region corresponds to atomic distances ($zp_F \sim 1$). The right-hand side of the curve is a plateau corresponding to independent, spatially-separated states. The characteristic scale $z_0 = 2l\ln(8/\nu)$.

spatial behavior of the correlator (1), whose general form follows from the foregoing and obvious physical considerations. In the figure, the point $z = x' - x = 0$ corresponds to the expression (4'); the hatched region, to atomic distances, i.e., to distances for which $p_F z \sim 1$, where the answer depends on the specific model. Further, the behavior of the correlator (7) smoothed out over atomic distances is depicted. At small distances (as compared to l, i.e., for $z \ll 1$) the behavior of the curve is determined by its value at zero value of its argument,

$$F_\omega(0) = \frac{\pi}{v_F^2}\int_0^\pi w(\theta)\, w(\pi-\theta)\, d\theta, \tag{10}$$

and the slope (first derivative)

$$\frac{dF_\omega}{dz}(0) = -\frac{\pi}{v_F^2}\int_0^\pi w(\pi-\theta)\,\frac{\partial}{\partial\theta}\,(w(\theta)\sin 2\theta)\, d\theta. \tag{10'}$$

The equality (10) follows from (9') and (7), while (10') is a consequence of Eq. (9) above and Eq. (39) in Ref. 7 for the steady-state phase distribution function $w(\theta)$. (Notice that the symbol ν used in Ref. 7 differs by a factor of 2 from the one used in the present paper.)

As z increases, the function $F_\omega(z)$ falls off (for sufficiently small ν). This decrease reflects the repulsion of levels with sufficiently close energies. At large distances the correlator (1) must go over into a product of densities of states:

$$F_\omega(z \to \infty) \approx (\pi v_F)^{-2}, \tag{11}$$

which corresponds to independent spatially-distant states of the one-dimensional chain.

Of primary physical interest is the correlation of two energetically close levels, i.e., levels for which $\nu \ll 1$, which we shall assume below to be fulfilled. In this case we have

$$F_\omega(0) = {}^2/_3(\pi v_F)^{-2}, \tag{12}$$

$$F_\omega'(0) = -{}^2/_3(\pi v_F)^{-2}. \tag{12'}$$

To find the general dependence on z, let us go over in (9) to the Laplace transforms in the coordinate z:

$$g_\omega(z, \theta) = \frac{1}{2\pi i}\int_{\delta-i\infty}^{\delta+i\infty} e^{\varkappa z}\,\tilde{g}_\omega(\varkappa, \theta)\, d\varkappa. \tag{13}$$

With allowance for (9') we obtain in place of (9) an equation for the transform:

$$\frac{\partial}{\partial\theta}\left(\sin^2\theta\frac{\partial}{\partial\theta}\tilde{g}_\omega\right)-\nu\frac{\partial}{\partial\theta}\tilde{g}_\omega-\varkappa\tilde{g}_\omega=-w(\theta). \tag{14}$$

This equation cannot be solved in closed form. It is well known,[7] however, that, for small ν, the function $w(\theta)$ is large in the domain of variation of the phase close to zero, i.e., for $\theta\sim\nu$:

$$w(\theta)\approx(1/\nu)\,w_0(\theta/\nu),\quad \theta\sim\nu,$$

and in the region close to π:

$$w(\theta)\approx w_1((\pi-\theta)/\nu),\quad \pi-\theta\sim\nu$$

(see the formulas (41)-(43) in Ref. 7). Therefore, it follows from the representation of F_ω in the form (7) that we shall also need for what follows the expression for $\tilde{g}_\omega$ in the same regions. Let us recall that the function $\tilde{g}_\omega$ is a periodic function with period π:

$$\tilde{g}_\omega(\varkappa,0)=\tilde{g}_\omega(\varkappa,\pi). \tag{15}$$

Thus, for small ν, the mathematical aspect of the problem consists in the solution of Eq. (14) in the regions of θ values close to zero and π and the matching of the solutions with the aid of the periodicity condition (15). In the region of small θ we have in place of (14) the equation

$$\frac{\partial}{\partial\theta}\left(\theta^2\frac{\partial\tilde{g}_\omega}{\partial\theta}\right)-\nu\frac{\partial\tilde{g}_\omega}{\partial\theta}-\varkappa\tilde{g}_\omega=-w(\theta) \tag{16}$$

(and similarly for $\pi-\theta\ll\pi$). The solution to Eq. (16) in this region can be expressed in terms of the modified Bessel functions:

$$\xi^{1/2}e^{-\xi}\{K_\mu(\xi),\ I_\mu(\xi)\}, \tag{16'}$$

where

$$\mu=(^1/_4+\varkappa)^{1/2},\quad \xi=\nu/2\theta.$$

In the main region $\theta\sim 1$ we can neglect the term $\nu\partial\tilde{g}_\omega/\partial\theta$ in (16), which yields

$$\frac{\partial}{\partial\theta}\left(\sin^2\theta\frac{\partial}{\partial\theta}\tilde{g}_\omega\right)-\varkappa\tilde{g}_\omega=-w(\theta). \tag{17}$$

The solution to Eq. (17) can be expressed in terms of the Legendre polynomials[10]:

$$(\sin\theta)^{-1/2}P_{1/2}^{\mu}(\cos\theta);\quad (\sin\theta)^{-1/2}P_{1/2}^{-\bar{\mu}}(-\cos\theta). \tag{18}$$

The solutions should be matched in the region

$$\nu\ll\theta\ll 1\quad(\nu\ll\pi-\theta\ll 1).$$

In this region the asymptotic forms of the functions (16') and (18) coincide, and have the form

$$\theta^{-1/2+\mu},\quad \theta^{-1/2-\mu}. \tag{19}$$

For correct matching to be possible, i.e., in order that the coefficients can be determined, the quantity $\mathrm{Re}\,\mu$ should, as we shall see, satisfy the condition

$$\mathrm{Re}\,\mu\leqslant 1. \tag{20}$$

Only in this case can both terms in (19) be separated against the background of the neglected term of the order θ^2 in (16) and the neglected terms with ν in (17). It is clear that the two terms in (19) are of the same order of magnitude for negative $\varkappa<-\frac{1}{4}$, i.e., for imaginary $\mu=(\frac{1}{4}+\varkappa)^{1/2}$.

We shall first investigate the solution to Eq. (14) in the general form, and then reduce the computation of the required quantities in the asymptotic regions to their determination under the condition (20).

It is in certain aspects convenient to rewrite Eq. (14), which is naturally solved as a standard second-order inhomogeneous equation if both solutions of the homogeneous equation are known, in terms of new variables in the infinite range $(-\infty,\infty)$, introducing for this purpose the variable $u=\cot\theta$ and a new function $\psi(u)$ defined by the relation

$$g_\omega(\varkappa,\theta)=e^{-\nu u/2}\psi(u). \tag{21}$$

For the function $\psi(u)$ we now have

$$-\psi''+\frac{\varkappa}{1+u^2}\psi+\frac{\nu^2}{4}\psi=\frac{w(u)}{1+u^2}e^{\nu u/2}\equiv f(u). \tag{22}$$

The left-hand side of (22) has the form of the Schrödinger equation (this transformation is noted also in Ref. 9) with potential

$$V(u)=\varkappa/(1+u^2) \tag{23}$$

and negative energy $-\nu^2/4$, which is small when $\nu\ll 1$. A characteristic of the potential (23) is its decrease at infinity according to the law u^{-2}, from which it follows, according to Ref. 11, that a system with such a potential will have an infinite number of levels when $\varkappa<-\frac{1}{4}$. Other boundary conditions for our problem (periodicity, Eq. (15)) do not allow us to express the solutions (22) in terms of the eigenfunctions of the quantum-mechanical problem, but the indicated circumstance manifests itself in rapid oscillations of the solutions for $\varkappa<-\frac{1}{4}$, which, by the way, is already evident from (19).

It is convenient to define the solutions to the homogeneous equation (14) in such a way that the first of them $g_1(\varkappa,\theta)$ is finite at the point π. It is easy to verify that the second linearly independent solution is

$$g_2(\varkappa,\theta)=e^{-\nu\,\mathrm{ctg}\,\theta}g_1(\varkappa,\pi-\theta). \tag{24}$$

The pair of independent functions $\psi_1(\varkappa,u)$ and $\psi_2(\varkappa,u)$ figuring in (22), and corresponding to this definition are uniquely determined by the requirement that ψ_1 decrease exponentially as $u\to-\infty$:

$$\begin{aligned}&\psi_1(\varkappa,u)\approx e^{\nu u/2}\quad(u\to-\infty),\\ &\psi_1(\varkappa,u)\approx C_1(\varkappa)e^{\nu u/2}+C_2(\varkappa)e^{-\nu u/2}\quad(u\to+\infty),\end{aligned} \tag{24'}$$

while the relation (24) corresponds to $\psi_2(u)=\psi_1(-u)$, which is a consequence of (21) and the evenness of the homogeneous part of Eq. (22) with respect to the substitution $u\to-u$. The Wronskian is equal to

$$\psi_1\psi_2'-\psi_1'\psi_2=-\nu C_1(\varkappa). \tag{25}$$

That solution $\psi(u)$ to the inhomogeneous equation (22) which satisfies the condition that $g_\omega(\varkappa,\theta)$ be finite at $\theta=0,\pi$ and also guarantees the fulfillment of the periodicity condition (15) has the form

$$\begin{aligned}\psi(u)=\frac{1}{\nu C_1(\varkappa)}\Big\{&\psi_1(u)\int_u^\infty\psi_1(-u')f(u')\,du'\\&+\psi_1(-u)\int_{-\infty}^u\psi_1(u')f(u')\,du'\\&+\frac{1}{C_1(\varkappa)-1}\psi_1(u)\int_{-\infty}^\infty\psi_1(-u')f(u')\,du'\Big\}.\end{aligned} \tag{26}$$

To the points where $C_1(\varkappa)=0$ correspond, according to (24), solutions of the Schrödinger equation (22) that decrease on both sides at $u=\pm\infty$. To such solutions would correspond a function $g(\varkappa,\theta)$ that does not satisfy the periodicity condition. It is easy to verify that, since $\psi_2(\varkappa,u)=\psi_1(\varkappa,u)$ for such $\varkappa$ values, the expression (26) as a function of $\varkappa$ actually does not have poles wherever $C_1(\varkappa)=0$. The singularities in the expression (26) as a function of $\varkappa$ are connected with the last term in it, or, more precisely, with the zeros of the denominator

$$C_1(\varkappa)=1, \tag{27}$$

which determine the eigenvalues and eigenfunctions of the non-self-adjoint boundary-value problem (14). The fact that the boundary points of the interval $(0,\pi)$ are both singular points imposes, on the face of it, mathematical limitations on the applicability of the results of the general theory (see, for example, Ref. 12). An analysis performed by us with a quasiclassical representation of the function $\psi_1(\varkappa,u)$ for large $|\varkappa|$ shows, however, that it is admissible to deform the contour for the $\varkappa$ integration in (23) into the left half-plane $\mathrm{Re}\,\varkappa<0$.

The next step consists in the use of the condition $\nu\ll 1$ to find in the region (20) an approximate expression for the function $g_1(\varkappa,\theta)$ (or $\psi_1(u)$) in the entire interval by matching the solutions to the homogeneous equation (14) or (22) near $\theta=0$ and $\theta=\pi$ (in the region $\nu\ll\theta\ll 1$). Such an operation can easily be performed, since the asymptotic forms of the solutions (16′) and (18) are well known.[10] Here we give only the final results. In the region $u\gg 1$ the function $\psi_1(\varkappa,u)$ has the form ($u'=\nu u/2$)

$$\psi_1(u)=C_1(\varkappa)\,(\pi/2)^{1/2}(u')^{1/2}[I_\mu(u')+I_{-\mu}(u')] +(2/\pi)^{1/2}\operatorname{ctg}\mu\pi\,(\gamma_\mu-\gamma_{-\mu})\,(u')^{1/2}K_\mu(u'), \tag{28a}$$

in the region $u<0, |u|\gg 1$ ($u'=-\nu u/2$)

$$\psi_1(u)=(2/\pi)^{1/2}(u')^{1/2}K_\mu(u'), \tag{28b}$$

and in the intermediate region $\nu|u|\ll 1$

$$\psi_1(u)=(\nu/\pi)^{1/2}(\sin\theta)^{-1/2}[A_\mu P_{\nu_h}^{\mu}(\cos\theta)+A_\mu' P_{\nu_h}^{-\mu}(-\cos\theta)]. \tag{28c}$$

Above we have used the notation:

$$\gamma_\mu=\frac{\Gamma(3/2-\mu)}{\Gamma(3/2+\mu)}\left[\frac{\Gamma(1+\mu)}{\Gamma(1-\mu)}\right]^2\left(\frac{8}{\nu}\right)^{2\mu}, \tag{29}$$

$$C_1(\varkappa)=[1-1/2(\gamma_\mu+\gamma_{-\mu})\cos\mu\pi]\sin^{-2}\mu\pi. \tag{30}$$

The constants A_μ and A_μ' are determined from the system

$$A_\mu\frac{\Gamma(\mu)}{\pi}=\frac{\pi}{2\sin\mu\pi}\frac{1}{\Gamma(1+\mu)}\left(\frac{\nu}{8}\right)^{\mu},$$

$$\frac{\pi}{2\sin\mu\pi}\frac{1}{\Gamma(1-\mu)}\left(\frac{8}{\nu}\right)^{\mu} \tag{31}$$

$$=A_\mu\frac{\Gamma(-\mu)}{\Gamma(3/2-\mu)\Gamma(-1/2-\mu)}+\frac{A_\mu'}{\Gamma(1+\mu)}. \tag{31′}$$

The expressions for A_μ and A_μ' will not be needed below, and their definitions (31) and (31′) are given in the form in which they figure in the matching conditions for the asymptotic forms for $\nu\ll\theta\ll 1$. Allowance for the higher-order terms from the expansion of $\sin^2\theta$ in powers of θ in (16) will give rise to corrections of relative magnitude ν^2 in (31) and (31′), whence we obtain the condition, (20), limiting the applicability of the matching procedure used.

We have already indicated above that the θ-integration domains near zero and π play the major role in (7). In fact, the expression for the relative order of magnitude of the quantity $w(\theta)$ in the region $\theta\sim 1$ contains an additional factor that is of the order of ν in smallness. Retaining in (7), (21), and (26) only the contribution from the principal regions, where the function $\psi_1(\varkappa,u)$ should, in its turn, be replaced by the expressions (28a) and (28b), rearranging the terms in (26) so as to get rid of spurious poles determined by the condition $C_1(\varkappa)=0$, and, finally, discarding all the terms that are analytic in the left half-plane $\mathrm{Re}\,\varkappa<0$, we obtain the following representation:

$$F_\omega(\varkappa)=\frac{\pi}{v_F^2}\frac{1}{\nu[C_1(\varkappa)-1]}\left(\int_{-\infty}^{\infty}f(u)\psi_1(-u)\,du\right)^2. \tag{32}$$

The integral in (32) is a sum of two terms $J^{(0)}$ and $J^{(\pi)}$, which contain contributions from the θ integration near zero ($u\gg 1$) and near π (u is negative and large), respectively.

Let us transform the denominator in (32) in accordance with (30) to the form

$$C_1(\varkappa)-1=\cos\mu\pi\sin^{-2}\mu\pi[\cos\mu\pi-\operatorname{ch}y(\mu)],\quad e^{y(\mu)}=\gamma_\mu. \tag{33}$$

So long as μ is small, we can, according to (29), use the expression

$$y(\mu)=2\mu L^*\approx 2\mu\ln(8/\nu). \tag{34}$$

The poles determined by the zeros of (33) correspond to a simple pole at $\varkappa=0$ ($\mu=\frac{1}{2}$) and two sets of complex-conjugate poles, which, for small μ (i.e., for $\varkappa$ close to $-\frac{1}{4}$), have the form

$$\mu_n^{(1)}=in\pi/(L^*+i\pi/2),\quad \mu_n^{(2)}=-in\pi/(L^*-i\pi/2). \tag{35}$$

The poles (35) consequently lie on both sides of the negative axis $\varkappa<-\frac{1}{4}$. The use of the set of eigenfunctions determined in accordance with (35) does not, however, offer any special advantage, and is useful only in the computation of certain asymptotic forms of little interest. The numerical computation of the behavior of the correlator (1) for, say, arbitrary $z=x-x'\sim 1$ requires the ability to evaluate the integral in (32) with rapidly oscillating eigenfunctions, the oscillations of these functions being connected with the specific nature of the potential $V(u)$, (23).

Having noted these mathematical characteristics, we proceed to directly compute (1) in the region $z\sim z_0$ (see Fig. 1), where strong repulsion occurs between two energetically close states in the case of small ν. We shall presently see that $z_0\sim\ln(1/\nu)\gg 1$ and, consequently, small $\varkappa$ values play a role in the representation (13). In (32) the dominant term is connected with $[J^{(0)}]^2$:

$$J^{(0)}=(1/4-\mu^2)/\cos\mu\pi\approx 1/\pi,\quad \mu\approx 1/2+\varkappa. \tag{36}$$

The expression (36) is the result of the integration of the function $w(\theta)\approx v^{-1}w_0(\theta/\nu)$, taken from (7), with (28b). We used the relation 6.621(3) from Ref. 13.

We should expand $\cos\mu\pi$ in the denominator of (32)

and take in (33) the dominant terms for small $\varkappa$:

$$F_\omega(\varkappa)=\left(\frac{1}{\pi v_F}\right)^2\frac{1}{\varkappa}\exp\left[-(2\mu-1)\ln\frac{8}{\nu}\right]$$
$$\approx\left(\frac{1}{\pi v_F}\right)^2\frac{1}{\varkappa}\exp\left[(-\varkappa+\varkappa^2)2\ln\frac{8}{\nu}\right].$$

The last expression should be substituted into the integral

$$F_\omega(z)=\frac{1}{2\pi i}\int_{\delta-i\infty}^{\delta+i\infty}e^{\varkappa z}F_\omega(\varkappa)\,d\varkappa,$$

in order to obtain the coordinate dependence of $F_\omega(z)$. Let us draw attention to the fact that the exponential function contains the combination $z-z_0$, where $z_0=2\ln(8/\nu)$, in view of which we have retained the terms quadratic in $\varkappa$ in the exponent in the preceding expression. The integration over $\varkappa$ is easy to perform. We see that, after a deep dip, the function $F_\omega(z)$, (1), begins to increase again in the vicinity of z_0:

$$F_\omega(z)=\frac{1}{(\pi v_F)^2}\left\{\frac{1}{2}+\frac{1}{2}\operatorname{erf}\left(\frac{z-z_0}{2z_0^{1/2}}\right)\right\}, \tag{37}$$

going over at $z<z_0$ into a product of two independent densities of states. The width of the transition region is

$$\Delta z\sim[\ln(8/\nu)]^{1/2}. \tag{37'}$$

It is of interest to compute the asymptotic law of decrease of the correlator (1) for small z in the left part of Fig. 1, i.e., for $1\ll z\ll z_0$. The term with $2J^{(0)}J^{(\pi)}$ in (32) is responsible for the corresponding variation, since the contribution from $[J^{(\pi)}]^2$ is everywhere small. In evaluating the integrals in $J^{(\pi)}$, which contain the expression

$$W_1(\theta)=W_1(u)=\frac{\nu|u|}{\pi^2}\int_0\frac{dt}{(1+t)^2}\exp(-\nu|u|t)$$

from Ref. (7) and Bessel functions, we found the formulas 6.622(3) and 7.512(10) in Ref. 13 useful. Let us, without going into the details of the computations performed, note that the answer can be obtained either by taking the residues (in the integration over $\varkappa$) at the poles (35) and then going over from summation to integration over $|\mu_n|\approx n\pi/L$ *, or by directly continuing the terms dominant with respect to ν in the region (20) with $\operatorname{Re}\mu>0$ to the $\varkappa<-\frac{1}{4}$ axis. Let us give the answer obtained in the indicated region:

$$F_\omega(z)=\frac{1}{(\pi v_F)^2}\frac{\pi^{1/2}}{16}\frac{e^{-|z|/4}}{|z|^{1/2}}. \tag{38}$$

This result differs by a numerical factor from the decay law found in Ref. 3 for the correlation of the moduli of the wave function of a single localized state at distances $|z|\gg1$. Thus, the wave functions of energetically close states almost coincide with each other at small distances. This does not contradict the ideas expressed in Ref. 1, according to which the wave functions of energetially close states are a result of the tunneling splitting of a pair of wave functions localized at two separate centers, with the important proviso, however, that the radius of localization in the problem in question is determined by the kinetic mean free path. Finally, let us, for completeness, give the correlator value, determined in accordance with (4'), at coincident points:

$$F_\omega(x'\equiv x)=(\pi v_F)^{-2}.$$

This value is exact, and does not depend on ν.

Let us say a few more words about the shape of the curve in the case when ν is not small. As ν increases, the dip gradually decreases, disappearing at $\nu\sim1$. At large ν the major part of the curve would correspond to a plateau (independent states). It is not difficult to obtain the corresponding small corrections in the correlator (1) at $\nu=\omega\tau\gg1$:

$$F_\omega(z)=\frac{1}{(\pi v_F)^2}\left[1-e^{-2z}\frac{\cos 2vz}{2v^2}\right].$$

These corrections, however, have over small distances an oscillating character, which reflects the beating of two energetically close wave functions.

3. ENERGY-LEVEL CORRELATION IN A FINITE CHAIN

The problem of the relative disposition of the energy levels in a fairly complex finite system was first formulated by Wigner[14] for nuclear levels. Its solution was subsequently offered by Dyson[15] in some general mathematical formulation. One of the formulations of the problem consists in the following. Let it be known that the mean level spacing is Δ. What is the probability of finding two levels a distance $E_2-E_1=\Delta$ apart if the interactions or the other parameters of the system can be considered to be random? It is suggested in Ref. 16 that it is precisely such a situation that, possibly, is realized for the electron levels in a small metallic particle containing scattering defects. Recently, Efetov[17] successfully demonstrated that the Dyson formulas are indeed reproduced in such objects.

In the one-dimensional case the density of states of a finite section (of length L) of a chain containing defects is

$$1/\Delta=L/\pi v_F. \tag{39}$$

A characteristic feature of the results obtained in Refs. 15 and 17 is the prediction of a significant correlation between levels over the energy range Δ. In the one-dimensional case we should rather expect the opposite assertion, since the energy levels are now connected with states localized at different points of the chain over a distance of the order of the mean free path $l\ll L$. Indeed, according to Refs. 8 and 9, the level distribution in this case is a Poisson distribution. We shall presently prove this assertion, using the formulas of the preceding section. Certain results obtained below supplement the results presented in Refs. 8 and 9.

Thus, we shall denote the correlator defined above by

$$S_\omega(x)=\left\langle\sum_{\mu\nu}\delta(E-\varepsilon_\mu)\,\delta(E+\omega-\varepsilon_\nu)\right\rangle, \tag{40}$$

where $\omega=E_2-E_1$. Rewriting the energy δ functions in terms of the phase δ functions and $d\phi/dE$, as is done in, say, Ref. 7, we introduce the function

$$S_\omega(x,\varphi,\theta)=\langle\delta(\varphi-\varphi_1^>)\,\delta(\theta-(\varphi_2^>-\varphi_1^>))\,\zeta_1^>\zeta_2^>\rangle. \tag{41}$$

The phases $\phi=\phi_1$ and $\theta=\phi_2-\phi_1$ pertain to the corresponding wave functions and for the present we regard the

chain length x as a variable. The phases are equal to zero at $x = 0$, and equal to integral multiples of π at $x = L$ if the states with energies ε_μ and ε_ν are eigenstates. The notation $\zeta = \partial\phi/\partial k$ was taken from Ref. 7. Similarly, $\phi_1^>$ and $\phi_2^>$ are that solution for the phases of the wave functions with energies E_1 and E_2 which satisfies the condition $\phi = 0$ at $x = 0$. The functions $\phi_1^>$ and $\phi_2^>$ increase monotonically with x and E ($\zeta^> > 0$ (Ref. 7)). In contrast to the preceding section where we considered an infinite chain, here it is expedient to refer the phase θ to the interval $(0,\pi)$. Therefore, the integral part of $[\theta^>(x)/\pi]$, i.e., the number of zeros of the wave function, directly indicates the number of levels lying in the interval between E_2 and E_1 along a section of the chain with length x. As to the phase ϕ, in the quasiclassical problem the phase with energy E_1 rapidly settles by itself into a steady-state distribution (over distances of the order of l). The brackets in (40) or (41) denote averaging over the various defect realizations in a finite segment and, hence, over the quasiclassical part of the energies E_1.

Besides the function $S_\omega(x,\phi,\theta)$, we must determine two other quantities:

$$\tilde{S}_\omega(x,\varphi,\theta) = \langle \zeta_1^> \delta(\varphi-\varphi_1^>)\delta(\theta-\theta^>)\rangle, \tag{42}$$

$$W_\omega(x,\varphi,\theta) = \langle \delta(\varphi-\varphi_1)\delta(\theta-\theta^>)\rangle. \tag{43}$$

Using the method of Ref. 7, we can easily derive the corresponding equation for each of these functions. Thus, we have

$$\frac{\partial w}{\partial x} = -\nu\frac{\partial w}{\partial\theta} + \frac{\partial^2}{\partial\theta^2}(\sin^2\theta w), \tag{44}$$

where, regarding the dependence on ϕ, we assume that the function $w_\omega(\phi,\theta) = w_\omega(x,\theta)$ has already settled into a steady-state distribution with respect to ϕ, and that it does not depend on this variable. Similar equations follow for $\tilde{S}_\omega$:

$$\frac{\partial\tilde{S}}{\partial x} = lw - \nu\frac{\partial\tilde{S}}{\partial\theta} + \frac{\partial}{\partial\theta}\left(\sin^2\theta\frac{\partial\tilde{S}}{\partial\theta}\right) \tag{45}$$

and $S_\omega(x,\theta)$ itself:

$$\frac{\partial S}{\partial x} = 2l\tilde{S} - \nu\frac{\partial S}{\partial\theta} + \sin^2\theta\frac{\partial^2 S}{\partial\theta^2}. \tag{46}$$

The boundary conditions for these equations are obvious:

$$w(x=0,\theta)=\delta(\theta), \quad \int_0^\infty w(\theta,x)\,d\theta = 1, \quad w(x,\theta\to\infty)=0. \tag{44'}$$

According to Ref. 7, $\zeta^>(x=0)=0$. It follows from the definitions (41) and (42) that

$$S_\omega(x=0,\theta)=\tilde{S}_\omega(x=0,\theta)=0, \quad \tilde{S}_\omega(\theta\to\infty,x)=0. \tag{45'}$$

With the aid of Eqs. (44)-(46) and these boundary conditions, we can easily verify the identities

$$\tilde{S}_\omega = -l\int_0^\theta \frac{\partial w}{\partial\nu}\,d\theta', \tag{47}$$

$$S_\omega = -l\int_0^\theta \frac{\partial\tilde{S}_\omega}{\partial\nu}\,d\theta' = l^2\frac{\partial^2}{\partial\nu^2}\int_0^\theta d\theta'\int_0^{\theta'} w\,d\theta''. \tag{48}$$

Thus, the problem has been reduced to the problem of determining the function

$$\Phi(x,\theta) = \int_0^\theta w_\omega(x,\theta')\,d\theta', \tag{49}$$

which, in its turn, satisfies the equation

$$\frac{\partial\Phi}{\partial x} = -\nu\frac{\partial\Phi}{\partial\theta} + \frac{\partial}{\partial\theta}\left(\sin^2\theta\frac{\partial\Phi}{\partial\theta}\right).$$

On account of (44'), the boundary condition for this equation is

$$\Phi(x=0,\theta)=1. \tag{44''}$$

Thus, the last equation differs from (9) only in that it has a different boundary condition, and that the domain of variation of θ is not limited to the interval $(0,\pi)$, but extends over the infinite interval $(0,\infty)$, reflecting the fact that, for a sufficiently long chain of length $L = x$, the number of levels in the energy range (E_1,E_2) is arbitrary. The physical meaning of the function $\Phi(x,\theta)$ consists, according to (49), in precisely the fact that the values of the function at the points $\theta = n\pi$ determine the probability of the system's having n levels in the chosen energy range. The function $\Phi(x,\theta)$ is a fundamental quantity for what follows. In the Laplace representation, the equation for its transform $\Phi_\varkappa(\theta)$ has the form

$$\frac{\partial}{\partial\theta}\left(\sin^2\theta\frac{\partial\Phi_\varkappa}{\partial\theta}\right) - \nu\frac{\partial\Phi_\varkappa}{\partial\theta} - \varkappa\Phi_\varkappa = -1. \tag{50}$$

The solution of (50) is

$$\Phi_\varkappa(\theta) = \varkappa^{-1} + \bar{\Phi}_\varkappa(\theta), \tag{51}$$

where in (51) $\bar{\Phi}_\varkappa(\theta)$ denotes that solution to the homogeneous equation in (50) which decreases as $\theta\to\infty$. In each interval $\theta_n = (n\pi,(n+1)\pi)$ the function $\bar{\Phi}_\varkappa$ is, as can easily be verified, directly expressible in terms of the function $g_1(\varkappa,\theta)$ (or $\psi_1(u)$) introduced in the preceding section by the formulas (24). In this case we have

$$\bar{\Phi}_\varkappa((n+1)\pi) = C_1^{-1}(\varkappa)\bar{\Phi}_\varkappa(n\pi), \tag{52}$$

and from the definition of $\Phi(x,\theta)$ for $x\neq 0$ it follows that $\Phi_\varkappa(\theta\to 0)\to 0$, i.e.,

$$\bar{\Phi}_\varkappa(\theta=0) = -\varkappa^{-1}. \tag{52'}$$

The formulas (52) and (52') constitute, in principle, the exact solution to the problem. But since we posed at the beginning of this section the question of level correlation under conditions when the characteristic energy scale $\omega = E_2 - E_1$ is comparable to the mean level spacing Δ, (39), of a large system, it is sufficient for this purpose to know all the quantities in the region $|\varkappa| \sim \nu \ll 1$. Carrying out the corresponding expansion in powers of $\varkappa$ in (29) and (30), we obtain

$$C_1^{-1}(\varkappa) \approx \frac{\nu}{\nu+\pi\varkappa}, \quad \bar{\Phi}_n(\varkappa) = \bar{\Phi}_\varkappa(n\pi) = -\frac{1}{\varkappa}\left(\frac{\nu}{\nu+\pi\varkappa}\right)^n. \tag{53}$$

Returning to the formulas (47)-(49), we find that the probability for a finite system of length $x = L$ to have n levels in the energy range ω is

$$w_n = (\nu x/\pi)^n e^{-\nu x/\pi}/n!. \tag{54}$$

In its turn, the condition for the absence of levels in this range is

$$w_0 = e^{-\varkappa x/\pi}. \quad (55)$$

Summation over all n gives the statistical number of levels in the range ω:

$$N_\omega = (L/\pi v_F)\,\omega. \quad (56)$$

The results (54)-(56) naturally coincide with the results obtained in Refs. 8 and 9, thus indicating the independence of the individual localized levels in the one-dimensional system. The expression for the correlator $S_\omega(x = L)$ has the form

$$S_\omega(L) = (\pi v_F)^{-2}[L - 2l \ln (8/\nu)]^2; \quad L > 2l \ln (8/\nu).$$

We should have more complete expressions if we left under the $\varkappa$-integration sign (in the inversion of the Laplace transformation) terms of the form

$$S_\omega(\varkappa) = \frac{l^2}{\pi\varkappa^2}\frac{\partial^2}{\partial\nu^2}\frac{\nu}{C_1(\varkappa)-1} \approx \left(\frac{l}{\pi}\right)^2 \frac{2}{\varkappa^3}\exp\left[2(-\varkappa+\varkappa^2)\ln\frac{8}{\nu}\right]. \quad (57)$$

Going over from $\varkappa$ to L (i.e., inverting the Laplace transformation), we find

$$S_\omega(L) = \frac{1}{(\pi v_F)^2}\int_0^L dx \int_0^x dx' \left[1+\operatorname{erf}\left(\frac{x'-x_0}{2(x_0 l)^{1/2}}\right)\right]; \quad x_0 = 2l\ln\frac{8}{\nu}.$$

These formulas are not given in Refs. 8 and 9. Notice that we already know from the results of the preceding section the estimate for the magnitude of the energy interval $\omega_0(L)$ in which there is, for a fixed chain length, appreciable level respulsion:

$$\omega_0 = (8/\tau)\,e^{-L/2l}$$

(here we have gone over to dimensional units, using the gas-kinetic definitions of the time interval between collisions and the mean free path). This estimate differs somewhat from the one given in Ref. 9 by numerical factors.

4. CONCLUSION

We have obtained the density-of-states correlation function for energetically close states in a one-dimensional chain which defects at different points. The result is represented in Fig. 1 by the curve, whose asymptotic behaviors are given by the formulas (37) and (38). This result is somewhat unusual in respect of that part of it (in the region $z \sim l$) which shows that two wave functions with close energies always overlap appreciably at distances $z \sim l$. (Attraction of levels!) And what is more, the expression (38) essentially shows that the two wave functions are virtually identical in the region $z \sim l$ prior to the onset of an irregularity or a dip, which reflects the fact that two electrons with nearly equal energies will, with high probability, occupy independent levels located far from each other. This circumstance is due to the fact that localization on defects is a complicated quantum-mechanical interference phenomenon, and that the localized state is centered on many defects at the same time. Nevertheless, the main results do not contradict the intuitive ideas. Moreover, the characteristic scale $z_0 = 2\ln(8/\nu)$ of the distances over which the interlevel interaction occurs is in accord with the tunneling estimates given in Ref. 1.

Our results also confirm the results obtained in Refs. 8 and 9 in respect of the statistical independence of the levels in a long segment of a linear chain containing defects. The general expression (57) allows us to find the level statistics for either small energy differences or shorter segments (but $l \ll L$).

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