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Density of states in a one-dimensional random potential

A. A. Ovchinnikov and N. S. Érikhman

L. Ya. Karpov Physicochemical Institute

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An exact expression is found for the density of energy states in a one-dimensional semiconductor having a narrow forbidden band in the presence of impurities. An equation of the Dirac type with a random Gaussian potential is chosen as a mathematical model for the description of such a system. It is shown that at low energies the density of states has the asymptotic form $\rho(E)\sim E^{\alpha}$ where the exponent α is a function of the impurity concentration. This dependence is used to explain the behavior of the paramagnetic susceptibility $\chi(T)$ at low temperatures in organic crystals of the NMP-TCNQ type.

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INTRODUCTION

The problem of the description of the energy spectrum in quantum one-dimensional (and quasi-one-dimensional) systems containing impurities is a timely problem. First of all because of the fact that even a small violation of strict periodicity in the one-dimensional case leads to an abrupt change in the nature of the system's spectrum, leads to localization of all eigenstates,[1,2] leads to the vanishing of the system's static conductivity,[3,6] and so forth. In this article we have investigated the energy spectrum of a system in the situation when the gap between two bands in a one-dimensional semiconductor is comparable in magnitude with a random field having a correlation function of the white-noise type. If the chemical potential of the system unperturbed by the random field is located in the middle of the forbidden band (this case occurs for example when the appearance of the gap is associated with the Peierls transition in a one-dimensional lattice), the density of energy states in the forbidden band determines such thermodynamic characteristics at low temperatures as the thermal conductivity, the magnetic susceptibility, etc. This connection is traced in detail in Ref. 7.

1. FORMULATION OF THE PROBLEM AND DERIVATION OF THE FUNDAMENTAL EQUATIONS

It is well known that a semiconductor with a narrow forbidden band can be described by an equation of the Dirac type[8]

$$-i\frac{\partial\psi_1}{\partial x}+\Delta(x)\psi_2=E\psi_1,\qquad i\frac{\partial\psi_2}{\partial x}+\Delta(x)\psi_1=E\psi_2,\tag{1}$$

where ψ_1 and ψ_2 represent the amplitudes of particles 1 and 2 moving to the right and to the left, $\Delta(x)$ is the potential for the interaction between particles 1 and 2. The functions $\psi_1(x)$ and $\psi_2(x)$ satisfy the periodic boundary condition:

$$\psi_1(0)=\psi_1(L),\quad \psi_2(0)=\psi_2(L).\tag{2}$$

In our case $\Delta(x)$ will be a random function of the form

$$\Delta(x)=\Delta_0+\xi(x),\tag{3}$$

where Δ_0 is a constant and $\xi(x)$ is a random field with correlation function ($\langle\ldots\rangle$ denotes the operation of statistical averaging)

$$\langle\xi(x)\rangle=0,\quad \langle\xi(x)\xi(y)\rangle=2D\delta(x-y). \tag{4}$$

It is necessary to solve Eq. (1) over the interval $(0, L)$ with the periodic boundary conditions (2). Instead of solving the system (1) for two complex functions ψ_1 and ψ_2, let us reduce (1) to a system of equations for two real functions. For this purpose we note that for any solution (ψ_1, ψ_2) of Eq. (1), a solution (ψ_2^*, ψ_1^*) exists with the same energy E. Let us form the sum and difference of these solutions:

$$\begin{pmatrix}\Psi\\ \Psi^*\end{pmatrix}=\begin{pmatrix}\psi_1+\psi_2^*\\ \psi_2+\psi_1^*\end{pmatrix},\quad \begin{pmatrix}\Phi\\ -\Phi^*\end{pmatrix}=\begin{pmatrix}\psi_1-\psi_2^*\\ \psi_2-\psi_1^*\end{pmatrix}. \tag{5}$$

It is obvious that the eigenfunctions (5) correspond to the same energy E. Let us introduce the new functions

$$f_1=\operatorname{Re}\Psi,\quad f_2=\operatorname{Im}\Psi,\quad \varphi_1=-\operatorname{Im}\Phi,\quad \varphi_2=\operatorname{Re}\Phi. \tag{6}$$

By substituting (6) into Eq. (5) and then into Eq. (1) we obtain the following system of equations for the functions f_1 and f_2:

$$\frac{df_1}{dx}=-(E+\Delta)f_2,\quad \frac{df_2}{dx}=(E-\Delta)f_1, \tag{7}$$

or

$$\hat{H}\begin{pmatrix}f_1\\ f_2\end{pmatrix}=\begin{pmatrix}\Delta, & \dfrac{d}{dx}\\ -\dfrac{d}{dx} & -\Delta\end{pmatrix}\begin{pmatrix}f_1\\ f_2\end{pmatrix}=E\begin{pmatrix}f_1\\ f_2\end{pmatrix}.$$

Exactly the same system of equations is obtained for φ_1 and φ_2.

Since the equations for (f_1, f_2) and (φ_1, φ_2) coincide, this implies that the spectra of the operators (1) and (7) are identical. For this reason it is sufficient to investigate the solution of the system (7). It follows from Eqs. (7) that every solution (f_1, f_2) with energy E has a corresponding solution (f_2, f_1) with energy $-E$, that is, the density of levels $\rho(E)$ is a symmetric function with respect to the point $E=0$. This property allows us to confine our attention to positive energies $E>0$ in the determination of $\rho(E)$. Before proceeding to the derivation of the fundamental equations, we note that the density of levels per unit length $\rho(E)$ does not depend on the boundary conditions as the system's length $L\to\infty$. Taking this property into consideration, we replace the periodic boundary conditions (2) by the following boundary conditions at the origin[1)]:

$$f_1(0)=f_1(L)=0. \tag{8}$$

One can easily verify that the operator (7) with condition (8) is Hermitian. Thus, the problem of determining the density of levels $\rho(E)$ of the system (1) reduces to finding the density of the spectrum of Eqs. (7) with the boundary conditions (8).

First let us consider the case when the field $\xi(x)=0$. In this case the solution of the system (7) corresponding to positive energy (as mentioned above, it is sufficient to consider only $E>0$) has the form

$$f_1=(E+\Delta_0)^{1/2}\sin[(E^2-\Delta_0^2)^{1/2}x],\quad f_2=-(E-\Delta_0)^{1/2}\cos[(E^2-\Delta_0^2)^{1/2}x]. \tag{9}$$

The boundary conditions (8) lead to the spectrum

$$E_n=(\Delta_0^2+\pi^2n^2/L^2)^{1/2},\quad n=1, 2,\ldots \tag{10}$$

Let us introduce the function $z(x)$:

$$z(x)=f_2/f_1. \tag{11}$$

From Eq. (9) we find that for $\xi(x)=0$

$$z(x)=\begin{cases}-\left(\dfrac{E-\Delta_0}{E+\Delta_0}\right)^{1/2}\operatorname{ctg}[(E^2-\Delta_0^2)^{1/2}x], & E>\Delta_0\\ -\left(\dfrac{\Delta_0-E}{\Delta_0+E}\right)^{1/2}\operatorname{cth}[(\Delta_0^2-E^2)^{1/2}x], & E<\Delta_0.\end{cases} \tag{12}$$

From Eqs. (8)–(10) and (12) it follows that the oscillation theorem is valid in the case $\xi(x)=0$: the number of the system levels in the energy interval $(0, E)$ is equal to the number of poles of the function $z(x)$ in the segment $(0, L)$. It is found that the theorem remains valid if the field $\xi(x)$ satisfies conditions (4) and as the system length $L\to\infty$. The proof is given in the Appendix.

Thus, to calculate the number of levels for the operator (7) it is sufficient to count the number of poles of the function $z(x)$. From Eqs. (7), (8), and (11) it follows that $z(x)$ satisfies the equation

$$\frac{dz}{dx}=(E-\Delta_0)+(E+\Delta_0)z^2+\xi(x)(z^2-1),\quad z(0)=-\infty. \tag{13}$$

The choice of the initial condition $z(0)=-\infty$ and not $z(0)=+\infty$ is dictated by the requirement for agreement with the case $\xi(x)=0$.

The function $z(x)$ is a functional of the field $\xi(x)$ and is therefore a random function. Its value at the point x is a random quantity whose density distribution is determined by the relationship

$$P(z, x)=\langle\delta(z-z(x))\rangle. \tag{14}$$

The probability density $P(z, x)$ satisfies the equation

$$\frac{\partial P}{\partial x}+\frac{\partial}{\partial z}\{[(E-\Delta_0)+(E+\Delta_0)z^2+2D(z^2-1)z]P\}-D\frac{\partial^2}{\partial z^2}[(z^2-1)^2P]=0. \tag{15}$$

The derivation of Eq. (15) utilizes the technique discussed in Refs. 9 and 10. This technique is based on the causality of Eq. (13), the correlation properties (4) of the field $\xi(x)$, and on the assumption concerning its Gaussian nature. The conditions enumerated here are assumed to be satisfied everywhere below.

Let us express the average number $\Pi_L(E)$ of poles of the function $z(x)$ in terms of the density $P(z, x)$ and its derivatives. $\Pi_L(E)$ is given by

$$\Pi_L(E)=\lim_{\lambda\to\infty}\left\langle\int_0^L\delta(\lambda-z(x))\frac{dz}{dx}dx\right\rangle. \tag{16}$$

In Eq. (16) we have substituted dz/dx in place of $|dz/dx|$. The reason is that the derivative $(dz/dx)|_{z=\lambda}$ is always positive as $\lambda\to\infty$ (see the Appendix). Substituting (13) into (16) we find

$$\Pi_L(E)=\lim_{\lambda\to\infty}\Big\{[(E-\Delta_0)+(E+\Delta_0)\lambda^2]\int_0^L dx\langle\delta(z(x)-\lambda)\rangle$$

$$+(\lambda^2-1)\int_0^L dx\langle\delta(z(x)-\lambda)\xi(x)\rangle\Big\}. \quad (17)$$

Taking (4) and the Gaussian nature of the process $\xi(x)$ into consideration, formula (17) can be rewritten in the following form:

$$\Pi_L(E)=\lim_{\lambda\to\infty}\Big\{[E-\Delta_0+(E+\Delta_0)\lambda^2]\int_0^L P(\lambda,x)\,dx$$

$$-D(\lambda^2-1)\frac{\partial}{\partial\lambda}\int_0^L dx\Big\langle\delta(z(x)-\lambda)\frac{Dz(x)}{D\xi(x)}\Big\rangle\Big\}. \quad (18)$$

The Gaussian nature of the field $\xi(x)$ was utilized in the transition from Eq. (17) to Eq. (18), this property being the one which permitted the application of relationship (10)

$$\int\langle\xi(x)F\{\xi(x)\}\rangle\,dx=\int dx\,dy\langle\xi(x)\xi(y)\rangle\Big\langle\frac{DF\{\xi(x)\}}{D\xi(y)}\Big\rangle.$$

The causality of Eq. (13) was also taken into consideration:

$$\frac{Dz(x)}{D\xi(y)}=0 \text{ for } x<y.$$

Taking the functional derivative of both sides of Eq. (13), we find

$$\frac{Dz(x)}{D\xi(x)}=z^2(x)-1.$$

Substituting this expression into formula (18) we obtain

$$\Pi_L(E)=\lim_{\lambda\to\infty}\Big\{[E-\Delta_0+(E+\Delta_0)\lambda^2]\int_0^L P(\lambda,x)\,dx$$

$$-D(\lambda^2-1)\frac{\partial}{\partial\lambda}(\lambda^2-1)\int_0^L P(\lambda,x)\,dx\Big\}. \quad (19)$$

In order to transform formula (19) into a more convenient form, we note that as $x\to\infty$ the solution $P(z,x)$ of Eq. (15) goes over into the function $P(z)$ which is the solution of a stationary equation of the following form:

Rp 653 $$\ )z^2-D(z^2-1)\frac{\partial}{\partial z}(z^2-1)\Big]P(z)\Big\}=0 \quad (20)$$

with the boundary condition

$$z^2P(z)\,|_{z=+\infty}=z^2P(z)\,|_{z=-\infty} \quad (21)$$

and the normalization condition

$$\int_{-\infty}^{+\infty}P(z)\,dz=1. \quad (22)$$

The choice of the boundary condition in the form (21) is explained in the Appendix. Taking Eq. (20) into consideration, from (19) we obtain the following expression for the number of poles per unit length $N(E)=\Pi_L(E)L^{-1}$ as $L\to\infty$:

$$N(E)=\lim_{z\to\infty}\Big\{(E+\Delta_0)z^2P(z)-D(z^2-1)\frac{\partial}{\partial z}[(z^2-1)P(z)]\Big\}. \quad (23)$$

Thus, in order to obtain the distribution function for the system's levels it is necessary to solve Eq. (20) with boundary conditions (21) and (22) and then evaluate the limit (23).

2. THE SOLUTION OF THE FUNDAMENTAL EQUATIONS AND THE CALCULATION OF THE DISTRIBUTION FUNCTION $N(E)$

By integrating Eq. (20) once we obtain

$$\frac{dQ}{dz}=\frac{1}{D(z^2-1)}\Big[\Delta_0+E+\frac{2E}{z^2-1}\Big]Q+\frac{C(E)}{D(z^2-1)}, \quad (24)$$

where

$$Q(z)=(z^2-1)P(z). \quad (25)$$

The constant $C(E)$ in Eq. (24) is chosen such that condition (21) is satisfied. The solution of Eq. (24) satisfying conditions (21) and (22) has the form

$$Q(z)=-(1+f(z))\Big/\int_{-\infty}^{+\infty}\frac{1+f(x)}{1-x^2}\,dx, \quad (26)$$

where the function $f(z)$ is given by

$$f(z)=\theta(z-1)\int_z^{\infty}F(y,z)\,dy+\theta(1-z^2)\int_z^{1}F(y,z)\,dy$$

$$+\theta(-z-1)\int_z^{-1}F(y,z)\,dy \quad (27)$$

($\theta(x)$ is the usual θ-function).

The function $F(y,z)$ is determined by the expression

$$F(y,z)=-[(\Delta_0+E+C_0)(y^2-1)+2E]\exp\Big[\frac{E}{D}\Big(\frac{y}{y^2-1}-\frac{z}{z^2-1}\Big)$$

$$+\frac{\Delta_0}{2D}\ln\Big|\frac{(z-1)(y+1)}{(z+1)(y-1)}\Big|\Big]\Big/D(y^2-1)^2, \quad (28)$$

and the constant C_0 in Eq. (28) is given by

$$C_0=-2D\Big/\int_0^{+\infty}\exp\Big[-\Big(\frac{\Delta_0}{2D}t+\frac{E}{2D}\operatorname{sh}t\Big)\Big]\,dt. \quad (29)$$

The quantity $C(E)$ in Eq. (24) is connected with the constant C_0 by the following relationship:

$$C(E)=-C_0\Big\{\int_{-\infty}^{+\infty}\frac{1+f(x)}{1-x^2}\,dx\Big\}^{-1}. \quad (30)$$

It is not difficult to verify that relationships (29) and (30) guarantee the fulfillment of conditions (21) and (22). Substituting (25) into (23) and taking (24) into consideration, we obtain the following relationship for the number of levels $N(E)$:

$$N(E)=-C(E). \quad (31)$$

The integral appearing in the denominator of formula (30) still has to be evaluated. By a change of variables of the form

$$\operatorname{sh} t=\frac{2z}{1-z^2},\quad \operatorname{sh}\tau=\frac{2y}{1-y^2}$$

this integral reduces to one found in the tables, and subsequently the following expression is obtained for the function $N(E)$:

$$N(E)=\frac{4D}{\pi^2\{J_\nu^2(E/2D)+N_\nu^2(E/2D)\}},\tag{32}$$

where $\nu=\Delta_0/2D$, and $J_\nu(x)$ and $N_\nu(x)$ are Bessel and Neumann functions.

In concluding this section we note that the described method can be used to evaluate the distribution function $N(E)$ for a system of the more general form

$$\begin{aligned}&-i\frac{\partial\psi_1}{\partial x}+\Delta_0\psi_2+\xi(x)\psi_2+\eta(x)\psi_1=E\psi_1,\\&i\frac{\partial\psi_2}{\partial x}+\Delta_0\psi_1+\xi(x)\psi_1+\eta(x)\psi_2=E\psi_2,\end{aligned}\tag{33}$$

where $\xi(x)$ and $\eta(x)$ are Gaussian random functions which are mutually independent. The correlation functions of the fields $\xi(x)$ and $\eta(x)$ are given by formula (4). In this case the function $N(E)$ has the form

$$\begin{aligned}N(E)=D\{1-\Phi^2(0,\infty)\}\Big/\Big\{&\int\limits_{-\infty}^{+\infty}R(x)\,dx\int\limits_{x}^{\infty}R(y)\Phi(x,y)\,dy\\&+\Phi^2(0,\infty)\int\limits_{-\infty}^{+\infty}R(x)\,dx\int\limits_{-\infty}^{x}R(y)\Phi(x,y)\,dy\Big\},\end{aligned}\tag{34}$$

where $R(x)=(x^4+2\gamma x^2+1)^{-1/2}$,

$$\Phi(x,y)=\exp\left\{\int\limits_{y}\frac{(E-\Delta_0)+(E+\Delta_0)z^2}{D(z^4+2\gamma z^2+1)}dz\right\}.$$

Here $\gamma=D_1/D_2$, $D=D_1+D_2$, and D_1 and D_2 denote the coefficients in the correlation functions of the field $\xi(x)$ and $\eta(x)$.

In the case when $\xi(x)=0$, formula (34) simplifies considerably and the expression

$$N(E)=D\left\{\int\limits_{-\infty}^{+\infty}dx\int\limits_{-\infty}^{x}dy\,\varphi(x)\varphi(-y)+(e^{\pi E/D}-1)^{-1}\left(\int\limits_{-\infty}^{+\infty}\varphi(x)\,dx\right)^2\right\}^{-1},\tag{35}$$

is obtained for $N(E)$ where

$$\varphi(x)=(x^2+1)^{-1}\exp\left[\frac{\Delta_0 x}{D(x^2+1)}-\frac{E}{D}\operatorname{arctg}x\right].$$

3. INVESTIGATION OF THE DEPENDENCE OF THE FUNCTIONS $N(E)$ AND $\rho(E)$ ON E AND ON THE PARAMETER $\nu=\Delta_0/2D$

For $E/2D\ll\nu$ expression (32) for $N(E)$ has the following asymptotic behavior:

$$\begin{aligned}N(E)&=\frac{4D}{\Gamma^2(\nu)}\left(\frac{E}{4D}\right)^{2\nu},\\\rho(E)&=\frac{dN}{dE}=\frac{2\nu}{\Gamma^2(\nu)}\left(\frac{E}{4D}\right)^{2\nu-1},\end{aligned}\tag{36}$$

where $\Gamma(\nu)$ is the Euler Γ-function. It is evident from Eq. (35) that when $E\to0$ the density of levels $\rho(E)\to0$ for $\nu>\frac{1}{2}$ and $\rho(E)\to\infty$ for $\nu<\frac{1}{2}$. One can show that a spectrum containing a pseudogap exists for $\Delta_0>D$, but for $\Delta_0<D$ the pseudogap is covered up. The authors of Ref. 11 arrived at an analogous result by using Brillouin-Wigner perturbation theory to second order in a similar problem.

For $\nu=0$, that is, $\Delta_0=0$, $N(E)$ and $\rho(E)$ take in the region of low energies the asymptotic forms

$$N(E)=\frac{D}{\ln^2(E/4D)},\quad\rho(E)=-\frac{2D}{\ln^3(E/4D)}.\tag{37}$$

Formulas (37) agree with the results obtained by Dyson in a special model.[12] It is a curious circumstance that for $\nu=\frac{1}{2}$ ($\Delta_0=D$) the influence of the gap is exactly cancelled by the presence of the irregularities, and $N(E)$ and $\rho(E)$ are given by

$$N(E)=E/\pi,\quad\rho(E)=1/\pi.\tag{38}$$

Let us trace the manner in which the transition occurs in the unperturbed case when $\nu\to\infty$ ($D\to0$). For $\nu\gg1$ the cylindrical functions in formula (32) admit of an asymptotic representation in terms of Bessel functions with index $\pm\frac{1}{3}$,[13] as a result of which the expression

$$N(E)=\frac{9D}{\pi^2w^2\{J_{-1/3}^2(\nu w^3/3)+J_{1/3}^2(\nu w^3/3)-J_{-1/3}(\nu w^3/3)J_{1/3}(\nu w^3/3)\}},\tag{39}$$

where $w=(E^2/\Delta_0^2-1)^{1/2}$, is obtained for $N(E)$.

In the case when $E<\Delta_0$ the Bessel functions in Eq. (39) are replaced by Bessel functions of imaginary argument. As $D\to0$ the parameter $\nu\to\infty$ and it follows from formula (39) that

$$N(E)=(E^2-\Delta_0^2)^{1/2}/\pi,\quad\rho(E)=E/\pi(E^2-\Delta_0^2)^{1/2}.\tag{40}$$

These expressions for $N(E)$ and $\rho(E)$ correspond exactly to the system's spectrum when the field $\xi(x)=0$ (see formula (10)). It is evident from (39) that at sufficiently high energies satisfying the condition

$$E^2\gg\Delta_0^2(1+\nu^{-2/3}),\tag{41}$$

the functions $N(E)$ and $\rho(E)$ are described by expression (40). In the narrow region

$$|E-\Delta_0|\lesssim\nu^{-2/3}\Delta_0\tag{42}$$

the function $N(E)$ has an inflection and $\rho(E)$ has a maximum given by

$$\rho_{max}=\frac{3^{2/3}\Gamma^3(2/3)}{2^{4/3}\pi^2\Gamma(1/3)}\nu^{1/3}.\tag{43}$$

For $E<\Delta_0$, just as follows from Eq. (39), $\rho(E)$ is exponentially damped with decreasing energy and only for $E\ll\Delta_0$, where the asymptotic form (39) is not valid, does the attenuation assume the power-law character (36). Thus we see that the presence of impurities smooths out the singularity in the function $\rho(E)$ for $E=\Delta_0$, converting it into a sharp maximum for $E\sim\Delta_0$. Let us note one more property of the distribution function $N(E)$. For a small value of the perturbing field $\nu\gg1$ ($\Delta_0\gg D$) the function $N(E)$ near the edge of the band,

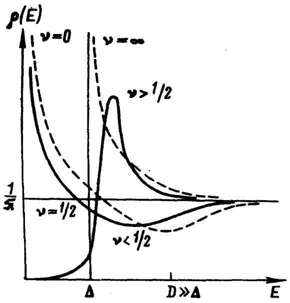

FIG. 1. Typical profiles of $\rho(E)$ as a function of the parameter ν for $D_2=0$.

that is, for $E\sim\Delta_0$ should have an asymptotic form corresponding to the usual Schrödinger equation.

In actual fact, at energies satisfying condition (42) formula (39) can be represented in the form

$$N(E)=\frac{(4D)^{1/3}\Delta_0^{2/3}}{\pi^2\{\mathrm{Ai}^2(-2\varepsilon)+\mathrm{Bi}^2(-2\varepsilon)\}}, \tag{44}$$

where

$$\varepsilon=(E-\Delta_0)(4D)^{-2/3}\Delta_0^{-1/3}$$

(Ai(x) and Bi(x) are Airy functions.[14]) If the value $(4D)^{-1/3}\Delta_0^{-2/3}$ is to be the unit of length, expression (44) identically coincides with the result obtained by Halperin.[15] Typical profiles of the function $\rho(E)$ are shown in Fig. 1 for different values of the parameter ν.

Now let us investigate the case when the system is described by Eq. (33) and $\xi(x)=0$. In this case $N(E)$ is given by formula (35). Analysis of this formula shows that for $E>\Delta_0\gg D$ the functions $N(E)$ and $\rho(E)$ are described by formulas (40), that is, they correspond to the unperturbed problem. The essential difference from the case analyzed above appears as $E\to 0$. It follows from Eq. (35) that as $E\to 0$ the level density $\rho(E)$ remains finite for arbitrary values of the parameter $\nu=\Delta_0/2D$:

$$\rho(0)=1/\pi I_0^2(\nu), \tag{45}$$

where $I_0(x)$ is the Bessel function of imaginary argument. Furthermore, $\rho'(0)=0$ for arbitrary ν, i.e., the function $\rho(E)$ has no discontinuities at zero in contradiction to the previous case when $\rho(E)$ had a discontinuity at zero for all $\nu<1$ (see Eq. (36)). In the situation when $\nu=0$ ($\Delta_0=0$) the influence of the gap is completely cancelled by the effect of the random field $\eta(x)$ and $\rho(E)$ is determined by formula (38) (in the case analyzed above, cancellation occurred for $\nu=\frac{1}{2}$). Profiles of $\rho(E)$ corresponding to $\xi(x)=0$ and $\eta(x)\neq 0$ are shown in Fig. 2.

Finally, let us present certain results which are valid in the general case when both fields, $\xi(x)$ and $\eta(x)$, are different from zero (see Eq. (33)). It is found that under these conditions the level density $\rho(E)$ remains finite as $E\to 0$ independently of the magnitude of the gap Δ_0. The corresponding expression for $\rho(E)$ is very cumbersome and we shall not write it down. However, this expression simplifies considerably for $\Delta_0=0$. In this case $\rho(0)$ is given by

$$\rho(0)=\frac{1}{\pi}\left(\frac{D_1+D_2}{D_2}\right)^{1/2}\Big/F^2\left(1/2,1/2,1,\frac{D_1}{D_1+D_2}\right), \tag{46}$$

where $F(\alpha,\beta,\gamma,x)$ is a hypergeometric function.

For $D_1=0$ Eq. (46) goes over into Eq. (38). For $D_2\to 0$ we obtain the following asymptotic expression for $\rho(0)$ from Eq. (46):

$$\rho(0)=\frac{\pi(D_1/D_2)^{1/2}}{\ln^2(D_1/D_2)}. \tag{47}$$

It is clear from this formula that the quantity $\rho(0)\to\infty$ as $D_2\to 0$, just as must also happen in the situation $\Delta_0=0$ and $\eta(x)=0$.

4. DISCUSSION

The results obtained above enable us to explain the experiments concerning the measurement of the paramagnetic susceptibility $\chi(T)$ at low temperatures for quasi-one-dimensional organic crystals of the NMP–TCNQ type. The experimental results cited in Ref. 7 indicate that at low temperatures $\chi(T)$ behaves like $T^{-\alpha}$ with $0<\alpha<1$. In order to explain such behavior of $\chi(T)$, the authors of the cited article made the assumption that the density of states $\rho(E)$ has a power-law singularity of the form $|E-E_F|^{-\alpha}$ at the Fermi surface with $0<\alpha<1$. The power-law behavior of $\chi(T)$ at low temperatures quickly follows from this assumption and from the fact that $\chi(T)$ has the form

$$\chi(T)=\frac{g^2\mu_B^2N}{2}\int_{-\infty}^{+\infty}dx\,\frac{\rho(E_F+2xT)}{\mathrm{ch}^2\,x} \tag{48}$$

as $T\to 0$. The described situation obviously holds in the case when total charge transfer occurs because in this connection the singularity in the level density arising from the impurities lies in the middle of the forbidden band and coincides with the Fermi level, which in the presence of impurities also occupies a position in the middle of the forbidden band.[2] Since in the model considered above the impurities lead to a power-law singularity in the level density $\rho(E)\sim E^{2\nu-1}$, the temperature dependence of the paramagnetic susceptibility will have the same form: $\chi(T)\sim T^{2\nu-1}$.

However, as is shown in Ref. 16 and is experimentally established in Ref. 17, an incomplete transfer of charge from donor to acceptor takes place in the organic crystals NMP–TCNQ and TTF–TCNQ. In this case the position of the Fermi level and the singularity in $\rho(E)$ do not coincide and the indicated mechanism for the appearance of the singularity in the paramagnetic susceptibility $\chi(T)$ as $T\to 0$ does not exist.[7] It is nevertheless possible that even in the presence of incomplete transfer of

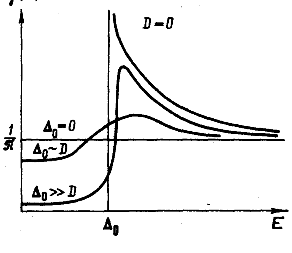

FIG. 2. Typical profiles of $\rho(E)$ as a function of the parameter ν for $D_1=0$.

charge, the impurities will be responsible for the appearance of a singularity in $\chi(T)$ at low temperatures. In actual fact let us describe the situation when there is a potential $V_0 \cos(k_F x)$ where k_F is the Fermi momentum (such a potential may appear), for example, in connection with the Peierls transition). In this case an intermixing of the electron's wave functions takes place at the Fermi surface and an energy spectrum arises containing a gap which has the following form near the edges of the band:

$$E_k = \pm(\Delta_0^2 + k^2)^{1/2}. \tag{49}$$

The spectrum (49) identically coincides with the spectrum of Eq. (1) in the absence of impurities ($\xi(x) = 0$) and therefore we have in essence the same situation as in the case of total charge transfer, that is, the Fermi level coincides with the position of the singularity in the density of states.

Thus we arrive at the conclusion that in the presence of incomplete charge transfer in the case of a Peierls transition, the presence of impurities in a one-dimensional organic crystal of the NMP–TCNQ type may lead to a power-law singularity $T^{-\alpha}$ in the temperature dependence of the paramagnetic susceptibility. It should also be noted that everything said above about the singularity in $\chi(T)$ is valid only for the case when impurities of a second type are not present ($\eta(x) = 0$) since for $\eta(x) \neq 0$ the functions $N(E)$ and $\rho(E)$ are finite as $E \to 0$ as is evident from Eqs. (34) and (35). Another consequence is the fact that for sufficiently regular crystals the behavior of $\chi(T)$ is not exponential as $T \to 0$ but instead obeys a power law $\chi(T) \sim T^{\alpha}$.

The results obtained for $\rho(E)$ possibly provide a model for understanding the experimental results concerning the paramagnetic susceptibility.[7]

In conclusion the authors express their gratitude to V. A. Onishchuk for a helpful discussion of the results.

APPENDIX

As is well known[9] a Gaussian random process $\xi(x)$ with the correlation properties (4) is the limit for a random process of the following form:

$$\xi_\beta(x) = \left(\frac{2D}{\beta}\right)^{1/2} \sum_{x_i} \theta_i \delta(x - x_i),$$
$$\xi(x) = \lim_{\beta \to \infty} \xi_\beta(x), \tag{A1}$$

where β is the average number of points x_i per unit length, θ_i are mutually independent random variables assuming the values ± 1 with probability $\frac{1}{2}$. The points x_i on the half-line $(0, \infty)$ have a Poisson distribution.

Let us consider the solution $z(x)$ of Eq. (13) with the potential $\xi_\beta(x)$. In this case the function $z(x)$ is a piecewise continuous function, and moreover in intervals of the form (x_i, x_{i+1}) it corresponds to the solution of the unperturbed problem ($D = 0$) and is described by formula (12) in which the initial phase of the cotangents must be properly chosen. From what has been said it immediately follows that $dz/dx > 0$ at points where $z(x) = \pm\infty$. This property was used in formula (16) of the main text. We further note that for almost any realization of the random function $\xi_\rho(x)$, i.e., with probability unity, the poles of the function $z(x)$ will lie inside intervals of the form (x_i, x_{i+1}). This means that the magnitude of the discontinuities of the function $z(x, E)$ at the points x_i will be a continuous function of the parameter E and therefore $z(x, E)$ will be continuous with respect to the totality of variables (x, E) inside any arbitrary interval (x_i, x_{i+1}). Hence it follows from the implicit-function theorem that the position of the poles $z(x, E) = \infty$ is a continuous function of the energy E because dz/dx is positive at the points corresponding to poles. The cited discussion gives a rigorous proof of the continuous dependence of the position of the poles of $z(x, E)$ on the energy E only for that case when the pole lies inside the interval (x_i, x_{i+1}). As for the poles which are encountered at the ends of the intervals $(x = x_i)$, the continuous dependence on the energy E holds for them only upon transition to the limit $\beta \to \infty$ since in this case the discontinuities of the function $z(x)$ at the points x_i tend to zero like $1/\beta^{1/2}$. Everything that has been said leads to the conclusion that the position of the n-th pole of the function $z(x, E)$ is a continuous, everywhere differentiable function of the energy $x_n(E)$ of the same type as the trajectory of Brownian motion.

The following two properties of the poles of the function $z(x, E)$ are essential for the proof of the oscillation theorem:

$x_n(E)$ is a continuous function of the energy, (A2)

$$z(x_n - 0) = +\infty, \quad z(x_n + 0) = -\infty, \quad n = 1, 2, \ldots \tag{A3}$$

It is easy to see that (A3) leads to the boundary condition (21).[3)] It follows from (A2) that upon a variation of the energy E the poles of the function $z(x, E)$ move continuously without any jumps along the x axis and each time when any pole crosses the point $x = L$, the corresponding energy E belongs to the spectrum of the operator (7). In the case of the ordinary Schrödinger equation, with increasing values of E the poles of $z(x, E)$ always move to the left; hence follows the oscillation theorem. In our case this is not so. However, the poles with sufficiently high numbers n do move to the left upon an increase of the energy E.

Let us prove this. Let us introduce random quantities $T_n(E)$ corresponding to the distances between neighboring poles

$$T_n(E) = x_n(E) - x_{n-1}(E). \tag{A4}$$

It follows from Eqs. (4), (13), and (A3) that the $T_n(E)$ are mutually independent, identically distributed random quantities. According to a well-known theorem of probability theory, the following relationship is valid for such quantities:

$$L(N) = \sum_{n=1}^{N} T_n(E) = NT(E)\{1 + O(N^{-1/2})\}, \tag{A5}$$

$$T(E) = \langle T_n(E) \rangle. \tag{A6}$$

The quantity $L(N)$ is the distance from the N-th pole to the point $x = 0$.

It follows from Eq. (A5) that for sufficiently large $N > N(E)$ the direction of motion of the N-th pole upon a variation of the energy is determined by the form of the function $T(E)$. Let us show that $T(E)$ is a monotonically decreasing function of the energy E. In actual fact, by inverting the function $L(N)$ from Eq. (A5) we obtain

$$N(L)=\frac{L}{T(E)}\{1+O(L^{-1/2})\}. \tag{A7}$$

We note that in Eq. (A7) the quantities $N(L)$ and $O(L^{-1/2})$ are random and depend on the specific realization of the field $\xi(x)$ whereas both the length L and the average distance $T(E)$ between the poles are not random quantities. Averaging both sides of Eq. (A7) and taking the limit $L\to\infty$ we obtain

$$T^{-1}(E)=\lim_{L\to\infty}\frac{\langle N(L)\rangle}{L}. \tag{A8}$$

The right-hand side of Eq. (A8) is none other than the monotonically increasing function $N(E)$ found above (see Eqs. (16), (23), and (32)) and consequently the inequality

$$\frac{dT}{dE}<0 \tag{A9}$$

is valid.

It follows from Eqs. (A5) and (A9) that poles with sufficiently large values of N move to the left upon an increase of the energy E. This implies that in the energy interval $(E, E+\Delta E)$ there will be just as many levels of the system as there are poles of the function $z(x, E)$ crossing the point $x=L$ upon a change of the energy from E to $E+\Delta E$.

Thus we arrive at the oscillation theorem in the following form: the number of the system's levels in the energy interval $(0, E)$ encountered per unit length of the system is equal, to within a constant which doesn't depend on the energy, to the density of poles of the function $z(x, E)$ when the length of the system $L\to\infty$. The constant mentioned in the formulation of the theorem is determined from the condition

$$N(E)=E/\pi \quad \text{as} \quad E\to\infty. \tag{A10}$$

In conclusion we note that in the case when $T(E) = N^{-1}(E)\to\infty$ as $E\to 0$ and the length of the system L remains finite, the oscillation theorem is inapplicable in the energy range $0<E\lesssim L^{-1}$ because at these energies a sufficiently large number of poles of the function $z(x, E)$ cannot be packed in the interval $(0, L)$.

1) The choice of boundary conditions in this form will be made clear later (see Eqs. (13) and (15)).

2) We have taken into consideration the fact that in the absence of impurities the lower band is completely occupied and the conduction band is empty.

3) More rigorously this is a consequence of the relationship.

$$\lim_{\varepsilon\to 0} z(x_n-\varepsilon)/z(x_n+\varepsilon)=-1.$$

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