# Density of states in a one-dimensional semiconductor with narrow forbidden band in the presence of impurities

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The density of the energy spectrum in a one-dimensional semiconductor with a narrow forbidden band is obtained in the presence of impurities.

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The problem of describing the energy spectrum of quantum one-dimensional and (quasi-one-dimensional) systems with impurities is still most pressing. The primary reason is that even a small deviation from strict periodicity leads in the one-dimensional case to an abrupt change in the character of the spectrum of the system, to localization of all the eigenstates, [1,2] to vanishing of the static conductivity of the system, [3–6] etc. We consider here the energy spectrum of a system under conditions when the gap between two bands in a one-dimensional semiconductor is comparable in magnitude with a random field having a correlator of the "white noise" type. If the chemical potential of the system unperturbed by the random field lies at the midpoint of the forbidden band (this case takes place, for example, when the apperance of the gap is due to a Peierls transition in the one-dimensional lattice), then the density of the energy states in the forbidden band determines at low temperatures such thermodynamic characteristics as the heat capacity, the magnetic susceptibility, etc. This connection is dealt with in detail in the review. [7]

It is known that a semiconductor with a narrow forbidden band can be described by the two-component Dirac equations[8]

$$\begin{cases} -i\dfrac{\partial\psi_1}{\partial x} + \Delta\psi_2 = E\psi_1 \\ i\dfrac{\partial\psi_2}{\partial x} + \Delta\psi_1 = E\psi_2, \end{cases} \tag{1}$$

where $\psi_1$ and $\psi_2$ are the amplitudes of particles 1 and 2, which move to the right and to the left, and $\Delta$ is the parameter of the interaction of particles 1 and 2. In our case $\Delta$ is a random function of $x$ in the form

$$\Delta(x) = \Delta_0 + \xi(x) \tag{2}$$

where $\Delta_0$ is a constant and $\xi(x)$ is a random field with a correlator ($\langle\cdots\rangle$ denotes the statistical-averaging operator)

$$\langle \xi(x) \rangle = 0, \quad \langle \xi(x)\xi(y) \rangle = 2D\delta(x-y). \tag{3}$$

The system (1) has solutions of two types: $\psi_2 = \psi_1^*$ and $\psi_2 = -\psi_1^*$. We choose, for example, the first case. We then obtain for the imaginary ($f_2$) and real ($f_1$) parts of $\psi_1$ the system of equations

  

$$\hat{H}\begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = \begin{pmatrix} \Delta(x), & \frac{d}{dx} \\ -\frac{d}{dx}, & -\Delta(x) \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = E\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}. \tag{4}$$

We choose the boundary conditions in a form

$$f_1(0) = f_1(L) = 0 \tag{5}$$

which ensures that the operator $\hat{H}$ is Hermitian. It must be emphasized that if $L$ is macroscopically large, the density of the energy spectrum does not depend on the form of the boundary conditions. Another possible form for them, for example, is $\psi_1(0)=\psi_1(L)$, $\psi_2(0)=\psi_2(L)$. We state without proof two most important properties of these equations: 1) The density of states $\rho(E)$ is an even function relative to the point $E=0$ under the conditions (2) and (3) and when $L$ is large (this can be easily verified, for example, by perturbation theory). 2) The number of states $N(E)$ in the energy interval from 0 to $E$ is equal to the number of zeros of the function $f_1$ in the interval $(0, L)$. This last statement is strictly valid for constant $\Delta(x)$, but if $\Delta(x)$ is subject to the conditions (2) and (3), it can be proved only if $L$ is sufficiently large (in contrast to the ordinary Schrödinger equation[9]).

The number of zeros of the function $f_1(x)$ or poles of the function $z(x)=f_2/f_1$ can be counted by writing out the equation for $z(x)$

$$\frac{dz}{dx} = (E-\Delta_0) + (E+\Delta_0)z^2 + \xi(x)(z^2-1) \tag{6}$$

and, using Halperin's method, obtain an equation for the function

$$P(z, x) = \langle \delta(z(x)-z) \rangle. \tag{7}$$

The principal equation takes the form

$$\frac{\partial P}{\partial x} + \frac{\partial}{\partial z}\{[(E-\Delta_0) + (E+\Delta_0)z^2 + 2Dz(z^2-1)]P\} - D\frac{\partial^2}{\partial z^2}[(z^2-1)^2 P] = 0. \tag{8}$$

It is obvious that $P(z,x)$ is independent of $x$ if $x$ is large, i.e., the function $N(E)$ is defined in terms of $P(z)$ in the following manner

$$N(E) = \lim_{z\to\infty}\left\{(E+\Delta_0)z^2 P(z) - D(z^2-1)\frac{\partial}{\partial z}[(z^2-1)P(z)]\right\}. \tag{9}$$

Equation (8) must be solved in the stationary state with two boundary conditions

$$\int_{-\infty}^{+\infty} P(z)dz = 1 \tag{10}$$

and

$$P(+\infty) = P(-\infty). \tag{11}$$

Omitting the intermediate calculations, we obtain

$$N(E) = \frac{4D}{\pi^2\{N_\nu^2(E/2D) + J_\nu^2(E/2D)\}}, \tag{12}$$

where $\nu=(\Delta_0/2D)$, $J_\nu$ and $N_\nu$ are Bessel and Neumann functions, respectively. The level density is expressed in terms of $N(E)$ in the usual manner, $\rho(E)$

$=N'(E)$. In the investigation of (12) a distinction must be made between the two cases $\nu<1/2$ and $\nu>1/2$, at which the density $\rho(E)$ exhibits a principally different behavior as $E\to 0$, namely $\rho(E)\sim|E|^{2\nu-1}\to 0$ for $\nu>1/2$ and $\rho(E)\sim|E|^{2\nu-1}\to\infty$ for $\nu<1/2$. It can thus be stated that at $\Delta_0>D$ we have a spectrum with a "pseudogap," and at $\Delta_0<D$ the "pseudogap" closes. It should be stated that a similar result was reached in[10], where Brillouin–Wigner second-order perturbation theory was used in a similar problem. We list the principal limiting cases of formula (12)

$$\rho(E)\sim\frac{-1}{|E|\ln^3|E|},\quad \nu=0;\quad \rho(E)\sim|E|^{2\nu-1},\quad 0<\nu<\infty;$$

$$\rho(E)=\frac{|E|}{\pi\sqrt{E^2-\Delta_0^2}},\quad \nu=\infty. \tag{13}$$

We note that at $\nu=0$ a similar singularity was obtained by Dyson[11] for the density of the spectrum exactly at the center of the band. The density $\rho(E)$ resumes its unperturbed value as $\nu\to\infty$. At lower $\nu$, the singularities in the density at $|E|\sim\Delta_0$ become smoothed out and are transformed into a maximum, the value at the maximum being $\sim\nu^{1/3}$. Approximate profiles for $\rho(E)$ at different values of $\nu$ are shown in Fig. 1. An unexpected feature is that at $\nu=1/2$ ($\Delta_0=D$) the effect of the gap is exactly canceled out by the presence of irregularities and we get $\rho(E)=1/\pi$, i.e., the value in the absence of an interaction of particles 1 and 2 with the impurity. Finally, in the case when the gap becomes very large, $\nu\gg 1$, and we are considering the behavior of the spectrum near the edge of the band, Eq. (12) goes into the expression obtained by Halperin, $\pi^{-2}[\mathrm{Ai}^2(-2\epsilon)+\mathrm{Bi}^2(-2\epsilon)]^{-1}$, where $\epsilon=E-\Delta_0$, Ai and Bi are Airy functions, with $(4D)^{2/3}\Delta_0^{1/3}$ chosen as the energy unit and $(4D)^{-1/3}\Delta_0^{-2/3}$ the length unit.

The foregoing results confirmed the hypothesis advanced in[7], that the lattice irregularities play a decisive role in the formation of the paramagnetic susceptibility $\chi(T)$ at low temperatures in the case of the quasi-one-dimensional organic crystals NMP-TCNQ. In contrast to,[7] the singularity of $\chi(T)$ as $T\to 0$ can occur for any degree of electron transfer from the donor to the acceptor,[12] i.e., at an arbitrary value of the chemical potential. Another consequence is that for sufficiently regular crystals the behavior of $\chi(T)$ as $T\to 0$ is not exponential but obeys the power law $\chi(T)\sim T^{2\nu-1}$.

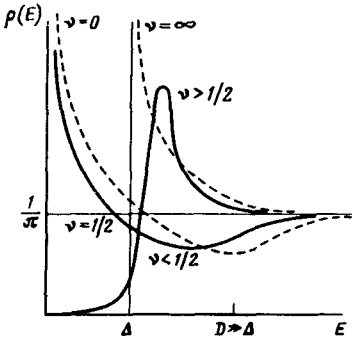


FIG. 1. Approximate density profiles $(E)$ as functions of the parameter $\nu=\Delta_0/2D$.

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