Metal-insulator transition in the anisotropy parameter in the case of a slight disorder

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Numerical calculations in a model with a weak impurity potential ($k_F l \gg 1$) reveal the point of a metal-insulator transition as the degree of quasi-one-dimensionality is increased.

At zero temperature in the one-dimensional ($1D$) case, an electron will be localized by an arbitrarily weak random potential if the interelectron interaction can be ignored. We thus run into the important question of whether a weak $1D$ localization ($k_F l \gg 1$) will be disrupted when account is taken of the small probability ($t_\perp$) that an electron will hop from one chain to another in the given quasi-one-dimensional ($Q\,1D$) compound. Whenever a result associated with $1D$ localization is used to describe a real physical phenomenon, it is actually being assumed implicitly that the phenomenon of weak $1D$ localization is stable with respect to the incorporation of a small probability $t_\perp$. On the other hand, if the anisotropy ($t_\parallel/t_\perp$), is not pronounced, the condition $k_F l \gg 1$ corresponds to a metallic phase. Consequently, if this assumption is correct, there must exist a point $(t_\perp)_c \ll t_\parallel$, at which a metal-insulator transition occurs. This transition was studied in Ref. 1 by a so-called self-consistent approach[2] to the theory of localization, and the value $2(t_\perp)_c = 0.31/\tau$, was derived, where $\tau = l/v_F$ is the kinetic mean free time. Although the estimate $(t_\perp)_c \sim 1/\tau$ seems plausible,[3] the very conclusion that there exists a transition at a finite $t_\perp$ apparently cannot be assumed proved, since the method[2] used in Ref. 1 is based on assumptions whose validity has not yet been established (a certain subset of the complete set of diagrams was summed in Ref. 2; the terms that were discarded were of the same order of magnitude as those that were retained).

In the present letter we report numerical calculations which provide unambiguous evidence in favor of a transition at

$$(t_\perp)_c = 0.08/\tau \tag{1}$$

under conditions such that we have $(t_\perp)_c \ll t_\parallel$.

We consider the standard model of a disordered $Q\,1D$ metal ($t_\parallel = 1$, $t_\perp \ll 1$) on a simple cubic lattice:

$$(\epsilon - U_{\mathbf{n}, n_z})\psi_{\mathbf{n}, n_z} = \psi_{\mathbf{n}, n_z - 1} + \psi_{\mathbf{n}, n_z + 1} + t_\perp \sum_{\mathbf{a}} \psi_{\mathbf{n}+\mathbf{a}, n_z}, \tag{2}$$

where $\mathbf{n} = (n_x, n_y)$; n_x, n_y, n_z are integers; $\mathbf{n} + \mathbf{a}$ corresponds to the four nearest neighbors of the vector $\mathbf{n}$; and the random potential U is specified independently at each site by means of the distribution function $P(U) = 1/W$ at $|U| < W/2$ and $P(U) = 0$ at

$|U| > W/2$. We fix the energy at the center of the zone ($\epsilon = 0$), and we consider only two values of the disorder: $W = 3.5$ and $W = 3.5/\sqrt{2}$. In each of these cases, the disorder can be regarded as weak, since the scale length over which the $1D$ localization [$\psi(z) \sim \exp(-|z|/\xi_{1D})$] develops is large, $\xi_{1D} = 105/W^2$.

Pichard and Sarma[4] have numerically determined the point of the Anderson transition in the isotropic case ($t_\perp = 1$) along the scale of the parameter W. Their result is $W_c = 19$. The method which they used[4] can be summarized as follows: The localization length ξ is first calculated in a long wire with a cross section $N \times N$, and then the question of whether $3D$ localization has occurred is answered by analyzing the function $\xi(N)$. Using the same method, we have studied the transition in the anisotropy parameter $t_\perp$ under conditions of a slight disorder. The result in (1) means that in the (W,$t_\perp$) plane there is a line which separates the metallic and insulating phases. The equation of this line at $t_\perp \ll 1$ is $t_\perp (3.5/W)^2 = 0.08$.

The localization length $\xi(N)$ is calculated for samples with the shape of a long bar ($L \gtrsim 3 \times 10^4$) with a cross section $N \times N$. The results are shown in Fig. 1, where the curves are labeled with the value of the parameter $A = 50t_\perp (3.5/W)^2$, and the crosses and the squares represent $W = 3.5$ and $W = 3.5/\sqrt{2}$', respectively. Obviously, the line which goes through the origin plays a very important role; this line corresponds to the value $A_c = 4$. The region $A \geqslant A_c$, where the localization length remains larger than the transverse dimension in the limit $N \to \infty$, should be identified with the

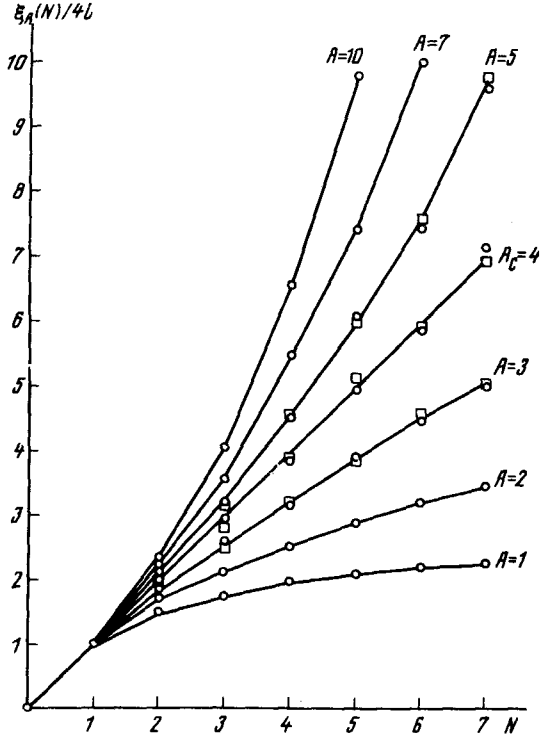

FIG. 1.

metallic phase. At $A < A_c$, on the other hand, the ratio $\xi(N)/N$ tends toward zero in the limit $N \gg 1$, as is characteristic of an insulating phase. It is natural to suggest that at $A < A_c$ the curves of $\xi_A(N)$ approach asymptotic values $\xi_A(\infty)$, but our calculations are not accurate enough for a determination of the exponent in the function $\xi_A(\infty) \sim (A_c - A)^{\nu}$.

Let us briefly outline the method used to calculate $\xi(N)$. For the $2N^2$-component vector

$$\Phi(L) = \begin{bmatrix} \psi_{n,L+1} \\ \psi_{n,L} \end{bmatrix}$$

we find the recurrence relation $\Phi(L) = m(L)\Phi(L-1)$ from (2), where the random symplectic matrix $m(L)$ is

$$m(L) = \begin{bmatrix} H(L) & -1 \\ 1 & 0 \end{bmatrix}, \tag{3}$$

$$H_{\mathbf{n},\mathbf{n}'}(L) = (\epsilon - U_{\mathbf{n},L})\delta_{\mathbf{n},\mathbf{n}'} - t_{\perp} \sum_{\mathbf{a}} \delta_{\mathbf{n}+\mathbf{a},\mathbf{n}'}. \tag{4}$$

We thus find

$$\Phi(L) = M(L)\,\Phi(0), \tag{5}$$

$$M(L) = \prod_{i=1}^{L} m(i). \tag{6}$$

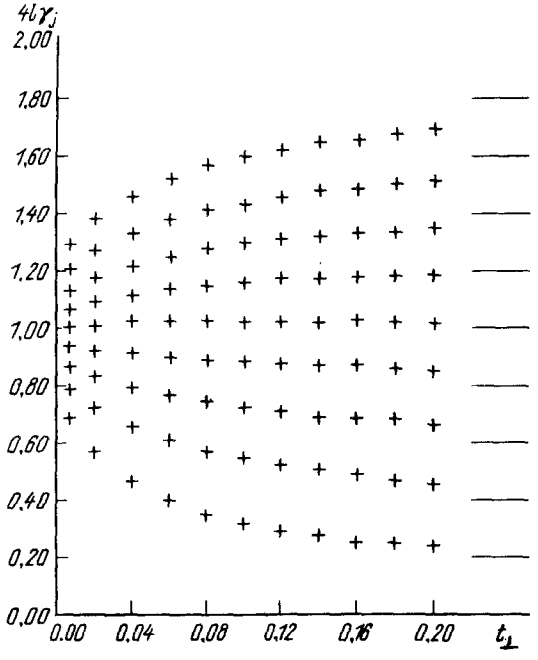

FIG. 2.

The localization of the wave function is obviously related to the rate of increase or decrease of $\Phi(L)$ with increasing L, while the change in $\Phi(L)$ is determined by the behavior of the eigenvalues of symplectic matrix (6). Half of the eigenvalues of this matrix, λ_j $(j = 1,...,N^2)$, grow exponentially $[\lambda_j = \exp(\gamma_j L)]$, while the remainder decay $[\lambda_{N^2+j} = 1/\lambda_j = \exp(-\gamma_j L)]$. The Lyapunov indices $0 < \gamma_1 < ... < \gamma_{N^2}$ are self-averaging quantities in the limit $L \to \infty$. The vector $\Phi(0)$ can be expanded in the eigenvectors of matrix (6), each of which decreases or increases in accordance with its own exponential function. In this manner, we obtain a hierarchy of scales $\xi_j = 1/\gamma_j$, as was pointed out in Refs. 3 and 5. A special role is played by the maximum scale, $\xi_1 = 1/\gamma_1$, which should be identified with the localization length $\xi(N)$.

Figure 2 shows a typical plot of the Lyapunov indices γ_j versus $t_\perp$ (we have chosen the parameter values $N = 3$ and $W = 3.5$). At $t_\perp = 0$ (the $1D$ case) there is a level degeneracy: $\gamma_j = 1/4l$, This degeneracy is lifted at $t_\perp \neq 0$. The average of the positive Lyapunov indices is expressed at the given $t_\perp$ in terms of the corresponding mean free path:

$$\langle \gamma \rangle = \frac{1}{N^2} \sum_1^{N^2} \gamma_j = (4l)^{-1} . \tag{7}$$

Shown at the right in Fig. 2 are the asymptotic values of the Lyapunov indices:

$$\gamma_j \left((t_\perp)_c \ll t_\perp \ll t_\parallel \right) = \langle \gamma \rangle \frac{2j}{N^2 + 1} . \tag{8}$$

Expressions (7) and (8) were derived in Refs. 3 and 5.

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