Localization and delocalization of particles in disordered lattice with tunneling amplitude with R^{-3} decay

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A renormalization procedure is used to analyze the problem of the localization of states in an Anderson model with a tunneling amplitude which decays over distance in accordance with R^{-3}. The result depends on the behavior of the distribution of the disordered potential at energies large in magnitude.

A particle undergoing a tunneling motion in a lattice with an energy disorder g_E^{-1} is known[1] to be localized if the amplitude for tunneling between sites, t_0, is small in comparison with the energy spread ($\chi_E = g_E t_0 \ll 1$). This conclusion is not valid if the tunneling $t_{\mathbf{R}}$ falls off slowly at large distances ($t_{\mathbf{R}} \propto R^{-\alpha}, \alpha \leqslant 3$). In the case $\alpha = 3$, the case of primary interest, we would expect a delocalization of all states, since for each site 1 with an energy E_1 the number of sites at resonance with it ($|E_2 - E_1| \lesssim |t_{12}|$) diverges logarithmically with distance from it.[1,2] In this case the standard description of delocalization runs into difficulty because it is not possible to construct an infinite cluster of resonant sites separated from each other by approximately the same distance.

We will use a renormalization procedure to study this problem.[2] In the first step, the tunneling is cut off at a certain scale R_0, and wave functions (R_0 modes) are constructed. In the next step, we choose a new cutoff scale $R_1 > R_0$, and new wave functions (R_1 modes) are constructed as a superposition of R_0 modes; etc. The small value of the parameter χ_t results in a localization of the wave functions in each step of the renormalization. To illustrate the point, we denote by R_i the cutoff radius at step i; $R_{i+1} = 2R_i$, $\chi_E = g_E t_0 \ln 2$. The increase in the localization radius l_i at step i occurs as a result of a resonance of the given state with states separated by a distance R, $R_i < R < R_{i+1}$. The probability for a "collision" with n resonances is $\chi_E^n \ll 1$. Consequently, the resonances collide in pairs, and we have $l_i \lesssim R_i$. The states delocalize only in the limit of an infinite cutoff radius; the particles propagate in accordance with a fractal law $\langle r \rangle \propto t^{1/3}$ (Ref. 2) (with $t_R = t_0/R^\alpha$, $\alpha < 3$, and an interatomic distance $\alpha = 1$, a delocalization of particles of energy E occurs if the cutoff radius satisfies $R_E \approx \chi_E{}^{1/(3-\alpha)}$. The description above is valid if the interaction constant t_0 is not renormalized.

We consider the case of a simple distance dependence of the tunneling: $t_R = -t_0/R^3$, $t_0 > 0$. We assume that we have two R_0 modes, with the annihilation operators $\psi^{(1)} = \Sigma_i u_i^{(1)} c_i$, $\psi^{(2)} = \Sigma_i u_i^{(2)} c_i$ (c_i are the site annihilation operators), separated by a distance R_1 which is greater than R_0 and greater than their localization radii. When the tunneling t_{R_1} is turned on, the overlap integral of $\psi^{(1)}$ and $\psi^{(2)}$ can be written in the form $v_{12} = -t_0 l^{(1)} l^{(2)}/R^3$, $l^{(p)} = \Sigma_i u_i^{(p)}$. We call the parameter $l^{(p)}$ the "length" of wave function $\psi^{(p)}$. We examine the renormalization of the lengths of the wave functions (i.e., the renormalization of the interaction constant).

The wave functions $\psi^{(1)}$ and $\psi^{(2)}$, with overlap v_{12}, are diagonalized by the standard transformation:

$$\tilde{\psi}^{(1)} = \cos\frac{\theta}{2}\,\psi^{(1)} + \sin\frac{\theta}{2}\,\psi^{(2)},\quad \tilde{\psi}^{(2)} = -\sin\frac{\theta}{2}\,\psi^{(1)} + \cos\frac{\theta}{2}\,\psi^{(2)},\quad \tan\theta = v_{12}/(E_1 - E_2). \tag{1}$$

In a corresponding way, we transform the parameters $l^{(1)}$ and $l^{(2)}$. The energies E_1 and E_2 vary in accordance with $E_{1,2} = (E_1 + E_2)/2 \pm (E_1 - E_2)/(2\cos\theta)$. We describe the effect of the renormalization procedure as a sequence of transformations (1). We introduce the distribution function of the states with respect to energy and length, $P(l,E,R)$, for a given cutoff radius R. The evolution of $P(l,E,R)$ with increasing cutoff radius, $P(l,E,R_1)-(Pl,E,R_0)$, is determined by the difference $[\delta(E-\tilde{E}_1)\delta \times (l-\tilde{l}_1) - \delta(E-E_1)\delta(l-l_1)]$, integrated over the number of collisions, d^3R, and also over the distributions of colliding states, $dl_1 dE_1 P(l_1,E_1,R) dl_2 dE_2 P(l_2,E_2,R)$. This approximation is applicable by virtue of the small value of the parameter $\chi_E^*(R) = t_0 \int P(l,E,R) l^2 dl$. If $\chi_E^*(R)$ is comparable to unity, then delocalized states with an energy E arise, and this description is no longer valid.

The renormalization equation is (cf. Ref. 2)

$$\begin{aligned} &P(l, E, R_1) - P(l, E, R_0) \\ &\quad = \int d^3\mathbf{R} \int dE_1 \int dl_1 \int dE_2 \int dl_2 P(l_1, E_1, R) P(l_2, E_2, R) \\ &\quad \times [\delta(E-\tilde{E}_1)\delta(l-\tilde{l}_1) - \delta(E-E_1)\delta(l-l_1)]. \end{aligned} \tag{2}$$

An important property of Eq. (2) is the conservation of $\langle l^2\rangle$ (if we multiply the right side by l^2 and integrate over $dldE$, we find zero). This property is a consequence of the orthogonality of transformations (1). That this property holds can be verified in the subsequent steps of the solution. For the quantity $\chi_E^*(R)$ in which we are interested, a leading role should be played by the nonresonant interaction with remote energies E_1 and E_2 (the resonance interaction does not change $\langle l_E^2\rangle$). The existence of this interaction can also be seen easily from first-order perturbation theory for $\langle l_E^2\rangle$. These arguments make it possible to restrict the analysis, in the switch to an equation for $\chi_E^*(R)$, to terms of first order in $\theta = v_{12}/(E_1 - E_2)$ [see (1)]. Multiplying (2) by l^2, integrating over dl, and taking the limit $R_1 \to R_0$, we find a closed equation for $\chi_E^*(\xi)$, $\xi = \ln R$:

$$\partial\chi_E^*/\partial\xi = -4\pi\chi_E^* \int dE_1 (E-E_1)^{-1}\chi_{E_1}^*, \quad \chi_E^*(0) = g_E t_0. \tag{3}$$

Equation (3) can be solved easily, since for a function of the complex variable $\psi_z = \int dE(z-E)^{-1}\chi_E^*$ we have $\partial\psi/\partial\xi = -2\pi\psi^2$. The solution is

$$\chi_E^*(\xi) = g_E t_0 |c_E|^2 |c_E + \xi|^{-2}, \quad c_E^{-1} = \int dE_1 (E - E_1 - i\delta)^{-1} g_{E_1} \cdot 2\pi t_0. \tag{4}$$

If the distribution falls off at high energies more rapidly than a Lorentzian distribution ($g_E \approx W^{\beta-1}/E^\beta, t_0 \ll W \ll E, \beta > 2$), then by selecting $E_0 \approx W(W/t_0)^{1/(\beta+2)}$ and $\xi_0 \approx E/2\pi t_0$ we obtain $\chi_{E_0}(\xi_0) \approx 1$, and delocalized states with an energy on the order of E_0 arise.

In the case of a slower decay of g_E ($1 < \beta \leqslant 2$), Eqs. (2) and (3) hold for arbitrary ξ, and the interaction constant is renormalized: $t_0(\xi) \propto \xi^{-2}$. All states are localized since the decay of the tunneling over distance is fairly rapid. If g_E is a Lorentz distribution, expression (4) becomes the same as the known exact solution for the corresponding Green's function,[3] $G(E,\mathbf{q}=0)$.

It is a simple matter to generalize (4) to the case of seed tunneling amplitudes of the type $t_0 l_1 l_2/R^3$ (l_i are random quantities), $t_0\mathbf{d}_1\mathbf{d}_2/R^3$ ($\mathbf{d}_i$ are random vectors), $t_0\cos(\mathbf{qR})/R^3$ ($\mathbf{q}$ is a constant vector), by simply changing the initial conditions for χ_E^* and for the parameter under study ($l_i \to \mathbf{d}_i; l^{(p)} \to \Sigma_i u_i^{(p)} \exp(i\mathbf{qR}_i)$). Accordingly, if the tunneling of excitations is characterized by an indirect interaction through conduction electrons (for example), intrinsic delocalized modes can exist in the system. This circumstance may have implications for the low-temperature thermal conductivity, etc.

Levitov[2] has used a renormalization equation like (2), for a time-independent distribution, to study the case in which tunneling is characterized by a dipole–dipole interaction. It was concluded from an analysis of a solution which is stationary with respect to ξ that the interaction constant is not renormalized. We believe the reason is the vanishing of the average of the tunneling amplitude over angles.

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