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The effect of disorder on the electronic states of two-dimensional systems

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Abstract. Under suitable approximations, it is shown that mobility of electrons in two-dimensional systems is always zero for a finite value of disorder, irrespective of the type of scattering potential.

1. Introduction

Two-dimensional 2D systems have attracted special attention in the study of certain transition phenomena as being the critical dimension between 1D and 3D whereby we can be certain that a transition occurs in three dimensions [1, 2] and does not in one [3, 4]. Usually one cannot reach a definite conclusion in two dimensions: considering for example the Anderson transition, while some authors state the existence of a transition [1, 5–7] some others claim that no transition exists [4, 8, 9]. It is believed that two dimensions bear inherent difficulties in nature, thus making the solution of the problem more intricate. In this connection one important work was carried out by Debney [1] who considered the completely disordered lattice by using the Ioffe–Regel condition $kL = 1$ where L is the mean free path, k is the wave vector. Denoting the ratio of Bohr radius a_0 to mean atomic separation a by x he found a transition at $x = 0.33$ in 3D and a transition at $x = 0.5$ in 2D. Though his result for 3D is in accordance with other work, the same cannot be said for the two-dimensional result $x = 0.5$ which falls opposite to physical expectations. Here one would expect that transition should take place much earlier than in the three-dimensional case because there is a general tendency that the transition point goes down as the dimensionality is reduced.

In [5–7] they used Hamiltonians with disordered site energies, and criteria for localization were different from those of [1]. In [5, 6] the effect of altering the system boundaries on a chosen energy-dependent quantity was employed in numerical studies, while in [7] the DC conductivity σ itself was computed by the memory function method.

According to [4] the current relaxation kernel $M(\omega)$ has the overall behaviour $M \propto -1/\omega$ with frequency in 2D for arbitrarily weak disorder, hence giving $\sigma = 0$ as $\omega \rightarrow 0$. Using scaling theory, Licciardello and Thouless [8] concluded that in 2D there might be complete localization even in the case of infinitely weak disorder (by analogy with the one-dimensional case). Later, by an extension of this work, the same conclusion was reached in [9].

In our previous work [10] we studied the three-dimensional completely disordered lattice model of Debney [1] and found that there was an Anderson transition at the point $x = 0.2$.

Owing to unsettled arguments on diverse results in 2D, at that time we left this case to a separate study which is the subject of this paper.

We showed that DC conductivity may be obtained as the limit of the real part of the frequency-dependent conductivity σ_r by [11, (2.2), (2.17)]

$$\sigma_r = \lim_{\omega \rightarrow 0} \frac{1}{V} \left(\frac{e}{m} \right)^2 \frac{\alpha_r(\omega)}{\omega^2} = \frac{1}{V} \left(\frac{e}{m} \right)^2 \frac{m^2 N^2}{6} \frac{\alpha_r''(0)}{(\alpha_r'(0))^2}. \quad (1.1)$$

Here $\alpha_r'(0)$ means $(\partial/\partial\omega)\alpha_r(\omega)$ evaluated at $\omega = 0$, and $\alpha_r''(0)$ is the second derivative defined in the same way. N is total number of free electrons, m is the electronic mass, e is the electronic charge and V is the volume of the system. $\alpha_r(\omega)$ is the real part of the force-force correlation function given by equation (2.15) of [11], which reads, after adapting to our model,

$$\alpha_r(\omega) = \frac{m^2 N^2}{(\alpha_r'(0))^2} \pi \hbar \sum_{k, k', q, q'} \delta(\hbar\omega - \Delta E') \frac{\langle [f_k^{*(1)}, f_k^{(1)}] \rangle_{\text{eq}}}{\Delta E'}. \quad (1.2)$$

Equations (1.1), (1.2) bear no approximations other than ω being small so they are valid under most general conditions like the Kubo conductivity formula. But due to the difficulties in the evaluation of commutator averages both in the numerator and in the denominator of equation (1.2) it is necessary to employ some approximation scheme. Equation (1.2) constitutes the starting point for our study from which one can obtain the following expressions for α_r' , α_r''

$$\alpha_r' = \frac{2\pi}{2N} \sum_{k, q} \hbar^2 q^2 |U_q|^2 n_k' \delta'(\Delta E') \quad (1.3)$$

$$\alpha_r'' = -\frac{2\pi\hbar}{2N} \hbar^2 q^2 |U_q|^2 n_k'' \delta''(\Delta E'). \quad (1.4)$$

Here n_k' is the derivative of electron occupation number n_k with respect to unperturbed energy E_k and $\Delta E'$ is the energy difference $E_{k+q} - E_k$. δ' , δ'' are the first and second derivatives of the Dirac delta functions (for details see [11]). On carrying out k, q sums both α_r' , α_r'' are seen to be proportional to N , therefore mobility

$$\mu = \frac{1}{6} e N \frac{\alpha_r''}{(\alpha_r')^2} \quad (1.5)$$

is independent of N . In our later calculations we left aside the factor N without causing any uncertainties.

2. The model Hamiltonian

Our model for two dimensions is the same as the one studied in [10] to find the Anderson transition. Since the details of this model were described fully in that work, here we are only going to recall necessary points. In the quasimomentum representation the system Hamiltonian $H = H_0 + U$ has the forms

$$H_0 = \sum_k H_{kk} c_k^\dagger c_k \quad (2.1)$$

$$U = \sum_{kq} H_{k+q, k} c_{k+q}^\dagger c_k \quad (2.2)$$

where $H_{k'k} = \langle k'|H|k \rangle$, $k' = k + q$, and c_k^\dagger , c_k are creation and annihilation operators for the electrons. The force component $f_k^{(1)}$ is given by $f_k^{(1)} = -iq_x U_q c_{k+q}^\dagger c_k$. If the diagonal elements H_{kk} were not configuration dependent they would correspond to E_k energy values as in the case of a regular lattice. The departure of the system from its unperturbed state is shown by the term $|U_q|^2$. In the quasimomentum representation energy E_k has no definite meaning in the sense of a dispersion relation because of configuration dependence. So, as in our previous work, we have taken a parabolic E_k dependence on k for the $\Delta E'$ appearing in equations (1.3), (1.4). For the 2D case Debney [1] gives $|U_q|^2$ to be

$$|U_q|^2 = \frac{1}{2} \mathcal{E}_k^2 + \frac{1}{2} \mathcal{E}_{k'}^2 + \frac{6}{8} \mathcal{A}^2 + \mathcal{A}^2 \frac{6 + \frac{1}{4} a_0^2 |\mathbf{k} + \mathbf{k}'|^2}{8[1 + \frac{1}{4} a_0^2 |\mathbf{k} + \mathbf{k}'|^2]^{7/2}}. \quad (2.3)$$

Note the existence of $\frac{1}{4}$ in front of $|\mathbf{k} + \mathbf{k}'|^2$ in $|U_q|^2$ expression above. We noticed that this $\frac{1}{4}$ factor is missing in our two previous work [10, 12] for 3D case. However we checked that our results were not influenced appreciably by this factor. In equation (2.3) \mathcal{E}_k has the meaning of an average energy

$$\mathcal{E}_k = \frac{\mathcal{A}^2}{(1 + a_0^2 k^2)^{5/2}} \text{Ryd}. \quad (2.4)$$

In fact this is the Fourier transform of the interatomic hopping potential averaged over different atomic sites with $\mathcal{A}^2 = 12\pi(a_0/a)^2$. If we want to define a coupling constant g to show the strength of disorder we can write $|U_q|^2 = g^2 |u_q|^2$, $g = x^2 = (a_0/a)^2$ and $|u_q|^2$ is the same as expression (2.3) except a factor of g^2 has been taken out from the each term.

3. Evaluation of α'_r , α''_r

For the evaluation of α'_r , α''_r first we have to define what form n'_k will take which plays a decisive role in the final results. In equations (1.3), (1.4) we should take n'_k as a convergent series

$$n'_k = [1 + A'_k + A_k'^2 + A_k A_k'' + \dots] \delta(\varepsilon_k - \varepsilon_F) \quad (3.1)$$

which is obtained from (14) and (31) of [12] (for details see the appendix). A_k is given by

$$A_k(\omega \rightarrow \mathcal{A}^2) = \frac{g^2}{N} \sum_{k' < k_F} \frac{|u_q|^2}{\omega - \varepsilon_{k'}}. \quad (3.2)$$

If this expression is evaluated in 3D it is easily seen to converge [10, 12], however the same expression diverges in the 2D case, as $\omega \rightarrow \mathcal{A}^2$

$$A_k \simeq \frac{S}{(2\pi)^2} \frac{2\pi}{N} g^2 |u_q|^2 \int_0^{k_F} \frac{k' dk'}{\omega - \varepsilon_{k'}} = \infty. \quad (3.3)$$

Using $S/N = a^2$ we see that A_k and its derivatives are also proportional to g and can be written as

$$A_k = g |u_q|^2 I(\omega) \quad (3.4)$$

by considering the divergent integral $I(\omega)$ to be finite

$$I(\omega) = \frac{a^2}{2\pi} \int_0^{k_F} \frac{k' dk'}{\omega - \varepsilon_{k'}} \quad (3.4a)$$

before the limiting case $\omega \rightarrow \mathcal{A}^2$. If we use the n'_k expression in (1.3) and (1.4) we find

$$\alpha'_r = \frac{2\pi}{N} [1 + A'_k + A_k^2 + \dots] g^2 \sum_{k,k'} (\hbar^2 k^2 + \hbar^2 k'^2 - 2\hbar^2 k k' \cos \phi) \times |u_q|^2 \delta(\varepsilon_k - \varepsilon_F) \delta'(\Delta E') \quad (3.5)$$

$$\alpha''_r = -\frac{2\pi}{N} [\dots] g^2 \hbar \sum_{k,k'} (\dots) |u_q|^2 \delta(\varepsilon_k - \varepsilon_F) \delta''(\Delta E') \quad (3.6)$$

where square and curved parentheses in equation (3.6) show the same terms as in equation (3.5). We have taken the square parentheses outside the sums in both of the equations above to make an approximation. We can do this because these parentheses are slowly varying functions of k . As we mentioned previously the integral $I(\omega)$ is so far kept finite, while the system disorder is in the vanishing limit $g \rightarrow 0$. All the calculations will be carried out under these assumptions and finally $I(\omega)$ will be taken to infinity. We saw that each of the sums in (3.5) and (3.6) gave finite values when carried out properly. So, we have $\alpha'_r = [\dots]C_1$, $\alpha''_r = [\dots]C_2$ with C_1, C_2 finite. Using these in the mobility expression we have

$$\mu \propto \frac{C_2}{[\dots]C_1^2}. \quad (3.7)$$

Since the square bracket expression contains powers of A_k, A'_k, A''_k it diverges in the $\omega \rightarrow \mathcal{A}^2$ limit where the integral $I(\omega)$ goes infinite. Because of the divergence of the square bracket in equation (3.7) the mobility becomes zero. The limiting value of $g \rightarrow 0$ corresponds to a small value of the disorder in the system where the mean separation between the atoms is large. Next we can say that higher values of g , corresponding to large disorder, will make the system mobility zero even more easily than the $g = 0$ case. Thus, within the present approximation we find that all the states are localized in 2D, which is in accordance with e.g. [9].

4. Discussion

Although equations (1.3), (1.4) for α'_r, α''_r contain $g^2 |u_q|^2$ this does not mean that they are the first terms in a perturbation expansion in g^2 . Rather they are exact, since equation (1.2) is exact from which they are derived for $\omega \rightarrow 0$. The commutator average in equation (1.2) $\langle [f_k^{*(1)}, f_k^{(1)}] \rangle_{\text{eq}}$ is calculated, by using the Vick's theorem, to be the difference of electron occupation numbers $n_k - n_{k+q}$. When divided by $\Delta E'$, this difference gives us the derivative of n_k with respect to energy, n'_k . The exact form of n_k is not known, but it should bear some resemblance to the Fermi function which is valid for the unperturbed system $n_k^0 = f(\varepsilon_k)$. In [12] it was shown that n_k and its derivatives should be treated as generalized functions whose value at a single point has no meaning. The form of n'_k , as derived from the imaginary part of the average Green function is given by equation (3.1). So, this equation relies very much on the averaging process that is applied to the Green function. As always some assumptions and approximations enter into the theory at this point, and because of these our n'_k expression may be said to be approximate. Otherwise there are no approximations in our α'_r, α''_r expressions.

At the beginning we mentioned that for 2D case there are two different views in the literature: one is saying that there is a transition and the other presages no transition at all. Our result supports the second view.

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Appendix

The electron occupation number n_k is obtained from equation (14) of [12]

$$n_k = -\frac{1}{\pi} \int d\omega G''_{kk}(\omega) f(\omega) \quad (\text{A1})$$

where G''_{kk} is the imaginary part of the Green function and $f(\omega)$ is the usual Fermi function. From equation (31) of [12]

$$G''_{kk}(\omega) = -\pi \delta(\omega - \varepsilon_k) + \pi \delta'(\omega - \varepsilon_k) A_k(\omega) - \frac{\pi}{2} \delta''(\omega - \varepsilon_k) A_k^2(\omega) + \dots \quad (\text{A2})$$

Using this expression in equation (A1) we obtain

$$\begin{aligned} n_k = & [1 + A'_k + A_k^2 + A_k A''_k + \dots] f(\varepsilon_k) \\ & + A_k [1 + A'_k + 3AA' + 3A^2A'' + 6AA^2 + \dots] \delta(\varepsilon_k - \varepsilon_F) \\ & + A_k^2 [1 + \dots] \delta'(\varepsilon_k - \varepsilon_F) + \dots \end{aligned} \quad (\text{A3})$$

which is considered in the convergent regime. As we mentioned in the text, A_k is proportional to g , which makes it small in the $g \rightarrow 0$ limit. While doing this we consider $I(\omega)$ to be finite (see equation (9)). The contents of the square brackets show similar structure but a factor of A_k appearing in front of any square bracket makes it small as compared with the first one. Therefore all the square brackets in equation (A3) may be dropped except the first. Applying the same ideas to the derivative of equation (A3) with respect to ε_k we obtain, after dropping the necessary brackets,

$$n'_k = [1 + A'_k + A_k^2 + A_k A''_k + \dots] \delta(\varepsilon_k - \varepsilon_F) \quad (\text{A4})$$

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