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The use of the correlation function technique for the Anderson transition

H Aktas, B Unal and B Alkan

Department of Physics, Faculty of Science, University of Ankara, 06100 Tandogan, Ankara, Turkey

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Abstract. For a completely disordered lattice, it is found that vanishing mobility is attained at a critical atomic density of $\rho_A^{1/3} a_0 = 0.2$, which agrees adequately with known results.

1. Introduction

The Anderson transition is a property of disordered conductors whereby the system goes from a metallic to an insulating state as the disorder is increased. To study this phenomenon one starts with a model of the conducting state in which the disorder may be due either to lattice irregularity (Matsubara and Toyozawa 1961) or site energies (Edwards and Thouless 1972) or both (Mott and Davis 1971). One chooses a parameter to measure the degree of each type of irregularity and changes the parameters to vary the randomness of the system.

There are different methods to study the transition regime such as looking at the mean free path L (Ioffe and Regel 1960, Debney 1976), using the $L(E)$ localization test (Economou and Cohen 1972), and using correlation function techniques which directly look at the transport coefficients (Vollhardt and Wolfle 1980, Gotze 1981). Calculating the transport coefficients from a suitable formula is a direct way to examine the above transition, since a vanishing value of the coefficient is indicative of the insulating state. Currently, new and practical formulae are being developed for transport coefficients (Milinski 1991, Unal *et al* 1992) and their capabilities should be tested through various applications.

In this work we apply the newly derived mobility formula of Unal *et al* (1992)

$$\mu = \tfrac{1}{2} e N \frac{\alpha_r''}{\alpha_r'^2} \frac{1}{3} \tag{1.1}$$

to a completely disordered lattice. Here e is the electronic charge, N is the total number of electrons and α_r', α_r'' are the frequency derivatives of the correlation function

$$\alpha(\omega) = \left\langle F_x \left| \frac{-j}{\omega - js - L} \right| F_x \right\rangle = \alpha_r(\omega) + j\alpha_i(\omega) \tag{1.2}$$

where

$$\alpha_r(\omega) = \pi \langle F_x | \delta(\omega - L) | F_x \rangle \tag{1.3}$$

$$\alpha_i(\omega) = -\left\langle F_x \left| \frac{1}{\omega - L} \right| F_x \right\rangle . \tag{1.4}$$

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In the above equations, L is the usual Liouville operator, ω represents frequency and F_x is the internal force related to the momentum P_x through $F_x = jLP_x$. It has been shown (Unal and Alkan 1993) that $\alpha_r(\omega)$ can be put into the form

$$\alpha_r(\omega) = -\frac{2\pi}{3}\sum_{kq}\hbar q^2|U_q|^2 n_k'\delta(\hbar\omega - \Delta E'). \tag{1.5}$$

The meaning of each term in this expression will be defined in the following sections.

The density of the medium, ρ_A, is considered in this paper to be the randomness parameter, and as we increase it we observe that the mobility drops to zero, thus giving the onset of the Anderson transition. As will be discussed later, the critical atomic density we obtain, $\rho_A^{1/3}a_0 = 0.2$, agrees reasonably with other estimates (Unal 1987, Debney 1976). We take this to be an indication that (1.1) works very well in this case.

Section 2 sets out the model Hamiltonian, section 3 is about the evaluation of α_r', α_r'' and section 4 deals with the transition density through an examination of μ. Finally, in the appendix we present detailed calculation of some integrals.

2. The model Hamiltonian

In this paper we consider the scattering of electrons in a metallic substance whose lattice site positions R_i have no regularity, which is known as a completely disordered lattice. Since this model is described fully elsewhere (Matsubara and Toyozawa 1961) we shall present here only an outline. Each atom is assumed to have an effective Bohr radius a_0 and is supposed to give a 1s electron to the medium. The mean atomic distance a is given by $a^3 = \Omega/N = \rho^{-1}$ where Ω and N show the volume and the number of atoms, respectively, and where ρ is the atomic density. In the quasi-momentum representation the system Hamiltonian $H = H_0 + U$ has the forms

$$H_0 = \sum_k H_{kk}C_k^+C_k \tag{2.1}$$

$$U = \sum_{kq} H_{k+q,k}C_{k+q}^+C_k \tag{2.2}$$

where $H_{k,k} = \langle k'|H|k\rangle$, $k' = k + q$, and C_k^+, C_k are creation and annihilation operators for the electrons. Using the same ideas as in a previous work (Unal 1987) we can replace the diagonal elements of H by their averages $\langle H_{kk}\rangle = (N/\Omega)V(k) = -\epsilon(k)$, where $V(k)$ is the Fourier transform of the interatomic hopping potentials and $\epsilon(k)$ is given by

$$\epsilon(k) = \frac{64(a_0/a)\pi}{(1 + a_0^2k^2)^3}\,\text{Ryd}. \tag{2.3}$$

Later in our calculation we shall need $\langle|H_{k'k}|^2\rangle = (1/N)|U_q|^2$, where $|U_q|^2$ is given by

$$|U_q|^2 = 2\epsilon_k^2 + 2\epsilon_{k'}^2 + \tfrac{7}{16}\mathcal{A}^3 + \mathcal{A}^3(7 + a_0^2|k + k'|^2)/16(1 + a_0^2|k + k'|^2)^4. \tag{2.4}$$

Here $\mathcal{A} = 4(a_0/a)\pi^{1/3}$ has been defined. The mobility equation contains the terms α_r' and α_r'', and we can write out these expressions, in our case, by comparing with similar

expressions in the work of Unal and Alkan (1993). Looking at their (2.6) and (2.7) we can write our α_r', α_r'' respectively as

$$\alpha_r' = \frac{2\pi}{3}\sum_{kq}\hbar^2q^2|U_q|^2n_k'\delta'(\Delta E') \tag{2.5}$$

$$\alpha_r'' = -\frac{2\pi}{3}\sum_{kq}\hbar^3q^2|U_q|^2n_k'\delta''(\Delta E') \tag{2.6}$$

where $\Delta E' = E_{k+q} - E_k$, n_k is the occupation number and n_k' stands for the derivative of the occupation number with respect to E_k. For reference purposes it has been necessary to use k vectors multiplied by $\hbar$, but in fact units where $\hbar = 1$ have been employed in this paper.

3. Evaluation of α_r' and α_r''

The sums in (2.5) and (2.6) may be evaluated by turning them into integrations in the usual way, by using the relations

$$\sum_q \to \frac{V}{(2\pi)^3}\int \mathrm{d}^3q \qquad \sum_k \to \frac{V}{(2\pi)^3}\int \mathrm{d}^3k.$$

If we denote the angle between the vectors k and q by α, with $\Theta = \pi - \alpha$, $\cos\Theta = \nu$, the energy difference $\Delta E'$ becomes

$$\Delta E' = -\frac{\hbar^2kq}{m}\nu + \frac{\hbar^2q^2}{2m}. \tag{3.1}$$

Integration is carried out in the order $\mathrm{d}\nu \to \mathrm{d}q \to \mathrm{d}k$ because, with this order, during the transformations of delta functions into simpler forms, Jacobians never become zero; otherwise, nothing fixes this order. The evaluation of α_r' and α_r'' are given in the appendix, and the results are

$$\begin{aligned}\alpha_r' = C_1\{&(1+\pi^2x^2)(1+4\pi^2x^2)^3[16+\tfrac{7}{128}(x/\pi)(1+\pi^2x^2)^6\\ &+\tfrac{1}{128}(1/\pi^3x)(1+\pi^2x^2)^6] - \tfrac{1}{256}(1/\pi^3x)[12\,288\pi^5x^3(1+4\pi^2x^2)^3\\ &+\tfrac{1}{16}(1+\pi^2x^2)(1+4\pi^2x^2)+\tfrac{7}{16}(1+4\pi^2x^2)^4+\tfrac{1}{2}](1+\pi^2x^2)^7\}\end{aligned} \tag{3.2}$$

$$\begin{aligned}\alpha_r'' = -C_2\{&960\pi^2x^2(1+4\pi^2x^2)^4+72\pi^7x^9(1+\pi^2x^2)^8-384(1+4\pi^2x^2)^4\\ &-[\tfrac{27}{64}(x/\pi)-2.625\pi x^3-12.25\pi^3x^5-7\pi^5x^7](1+\pi^2x^2)^8\}.\end{aligned} \tag{3.3}$$

Here C_1, C_2 are constants and x is a parameter defined as $x = a_0/a$. Using these expressions in (1.1) we may obtain the mobility, μ, as a function of x. When the mean interatomic distance a is large, corresponding to small values of x, the atoms in the system are far apart from each other and in this case we expect that the scattering of an electron should be weak. The mobility will then have a large value, but as the parameter x is increased the scattering of an electron with atoms will take place more effectively; therefore we may expect a decrease in the mobility. In order to check this expectation we looked at α_r'' appearing in the numerator of the mobility equation (1.1): α_r'' had a value of $384C_2$ for $x = 0$ and it decreased as we slowly increased the parameter x. The value of $x = 0.2$ was just enough to make α_r'' (and hence μ) zero. While doing these processes we observed that α_r' was never zero. We thus concluded that the entire system changed its state from a conducting to a non-conducting one: an Anderson transition took place.

4. Conclusions

As we mentioned in the introduction, there is currently a great deal of effort in developing new and practical formulae for the calculation of transport coefficients of condensed matter. These formulae differ from each other by the ease with which an actual computation can be carried out in particular applications. The correlation function technique of Vollhardt and Wolfle (1980) and of Gotze (1981) was used by one of us in a previous work and gave the result $\rho_A^{1/3} a_0 = x = 0.29$ (Unal 1987), but in this paper we use the mobility formula developed by Milinski (1991) and the corrected version developed by Unal *et al* (1992). The mobility formula has not been used before in the study of the Anderson transition for a completely disordered lattice model. In this respect our work aims to show the usefulness of the mobility formula for studying the Anderson transition. Using the Ioffe–Regel condition for the mean free path of electrons, Debney (1976) found that this transition took place at $x = 0.33$ while Fertis *et al* (1981) and Logan and Volynes (1985) obtained the values $x = 0.16$ and $x = 0.12$ respectively. Our result in this paper, $x = 0.20$, falls right inside the region subtended by the above values. This shows that the use of the mobility formula may constitute a basis for the study of the Anderson transition.

Appendix.

In order to evaluate α_r' the expressions of $|U_q|^2$ and $\Delta E'$, given by (2.4) and (3.1) respectively, are used in (2.5). For the n_k' term appearing in (2.5) we use the result

$$n_k' = \left[1 - \left(\frac{\mathrm{d}A}{\mathrm{d}\epsilon_k}\right)_{\epsilon_F}\right]^{-1} \delta(\epsilon_F - \epsilon_k) \tag{A.1}$$

obtained from (25) and (27a) of a previous work (Unal 1987) under the same approximations cited therein. Now α_r' becomes

$$\alpha_r' = -\frac{2\pi}{3}\sum_{kq}\hbar^2 q^2 \frac{1}{N}\left(2\epsilon_k^2 + 2\epsilon_k^2 + \tfrac{7}{16}\mathcal{A}^3 + \mathcal{A}^3 \frac{7 + a_0^2(4k^2 - 4kq\nu + q^2)}{16[1 + a_0^2(4k^2 - 4kq\nu + q^2)]^4}\right)\frac{m^2}{\hbar^2 k^2 \hbar^2 q^2}\delta'(\nu - \nu_0)\frac{\delta(\epsilon_F - \epsilon_k)}{1 - A'(\epsilon_F)}. \tag{A.2}$$

The term $\delta'(\Delta E')$ has been transformed as follows (Unal 1987):

$$\delta'\left(-\frac{\hbar k \cdot \hbar q}{m}\nu + \frac{\hbar^2 q^2}{2m}\right) = -\frac{m^2}{\hbar^2 k^2 \hbar^2 q^2}\delta'(\nu - \nu_0) \tag{A.3}$$

and since the root $\nu_0 = \hbar q/2\hbar k$ has to remain between 0 and 1 we have the limitation $\hbar q = 2\hbar k$ during the $\mathrm{d}q$ integral. A factor of 2π comes from the $\mathrm{d}\phi$ integral and thus we have

$$\alpha_r' = -\frac{2\pi}{3N}\frac{2\pi V m^2}{\hbar^3(2\pi)^3}\sum_k \frac{1}{\hbar^2 k^2}\frac{\delta(\epsilon_F - \epsilon_k)}{1 - A'}\int_0^{2\hbar k}\hbar^2 q^2\,\mathrm{d}(\hbar q)\int_0^1 \delta'(\nu - \nu_0)[.]\,\mathrm{d}\nu. \tag{A.4}$$

The notation [.] denotes all the contents of the square brackets in (A.2). Equation (A.4) becomes

$$\alpha_r' = -\frac{Vm^2}{3N\hbar^3\pi}\sum_k \frac{1}{\hbar^2k^2}\frac{\delta(\epsilon_F-\epsilon_k)}{1-A'}\int_0^{2\hbar k}\hbar^2q^2\,\mathrm{d}(\hbar q)\Bigg[\left(\frac{(64\pi a_0/a)^2}{(1+a_0^2k^2)^6}+14\pi(a_0/a)^3\right)$$
$$\times\delta(1-\hbar q/2\hbar k)+\int_0^1\frac{(64\pi a_0/a)^2}{[1+a_0^2(k^2-2kq\nu+q^2)]^6}\delta'(\nu-\nu_0)\,\mathrm{d}\nu$$
$$+2\pi(a_0/a)^3\int_0^1\frac{7+a_0^2(4k^2-4kq\nu+q^2)}{[1+a_0^2(4k^2-4kq\nu+q^2)]^4}\delta'(\nu-\nu_0)\,\mathrm{d}\nu\Bigg]. \tag{A.5}$$

Integration of the second and third terms inside the large square brackets is done by observing the rule

$$f(x)\delta'(x)=f(x_0)\delta'(x)-f'(x_0)\delta(x) \tag{A.6}$$

$$\alpha_r' = -\frac{Vm^2}{3N\hbar^3\pi}\sum_k \frac{1}{\hbar^2k^2}\frac{\delta(\epsilon_F-\epsilon_k)}{1-A'}\Bigg[\int_0^{2\hbar k}\hbar^2q^2\,\mathrm{d}(\hbar q)\left(\frac{(64\pi a_0/a)^2}{(1+a_0^2k^2)^6}+14\pi(a_0/a)^3\right)$$
$$\times 2\hbar k\,\delta(\hbar q-2\hbar k)+\frac{(64\pi a_0/a)^2}{(1+a_0^2k^2)^6}2\hbar k\int_0^{2\hbar k}\hbar^2q^2\,\mathrm{d}(\hbar q)\,\delta(\hbar q-2\bar{k})$$
$$-12a_0^2k\frac{(64\pi a_0/a)^2}{(1+a_0^2k^2)^7}\int_0^{2\hbar k}\hbar^3q^3\,\mathrm{d}(\hbar q)$$
$$+2\pi(a_0/a)^3\int_0^{2\hbar k}\frac{7+a_0^2(4k^2-q^2)}{[1+a_0^2(4k^2-q^2)]^4}\hbar^2q^2 2\hbar k\,\delta(\hbar q-2\hbar k)\,\mathrm{d}(\hbar q)$$
$$-24\pi(a_0/a)^3a_0^2k\int_0^{2\hbar k}\frac{9+a_0^2(4k^2-q^2)}{[1+a_0^2(4k^2-q^2)]^5}\hbar^3q^3\,\mathrm{d}(\hbar q)\Bigg]. \tag{A.7}$$

The $\mathrm{d}(\hbar q)$ integrals are easily carried out, and while doing $V/(2\pi)^3\int\mathrm{d}^3k$ integration we have to take into account the relation

$$\delta(\epsilon_F-\epsilon_k)=\frac{(1+a_0^2k_F^2)^4}{384\pi(a_0/a)a_0^2k_F}[\,\delta(\hbar k-k_F)+\delta(\hbar k+k_F)]. \tag{A.8}$$

After the $\mathrm{d}k$ integration we have to put $k=k_F$, and on putting $a=\pi/k_F$ we can arrange the whole expression in terms of the parameter $x=a_0/a$. The result is

$$\alpha_r' = \frac{Vm^2}{3N\hbar^3\pi^2}\frac{4\pi V}{(2\pi)^3\hbar^3}\frac{(1+\pi^2x^2)^4}{384(1-A')a_0^3}[\![16(64\pi x)^2(1+\pi^2x^2)\pi^2x^2(1+4\pi^2x^2)^3$$
$$+224\pi^3x^5(1+4\pi^2x^2)^3(1+\pi^2x^2)^7-48\pi^4x^4(64\pi x)^2(1+4\pi^2x^2)^3$$
$$-\pi x^3\{(9+4\pi^2x^2)[3(1+4\pi^2x^2)^4-4(1+4\pi^2x^2)^3+1]$$
$$-3(1+4\pi^2x^2)^5+\pi^2x^2(1+4\pi^2x^2)+8(1+4\pi^2x^2)^4$$
$$-6(1+4\pi^2x^2)^3\}(1+\pi^2x^2)^7]\!]/\pi^2x^2(1+4\pi^2x^2)^3(1+\pi^2x^2)^7. \tag{A.9}$$

To evaluate α_r'' we can transform the term $\delta''(\Delta E')$ in (2.6) as

$$\delta''\left(-\frac{\hbar k\hbar q}{m}\nu+\frac{\hbar^2q^2}{2m}\right)=\frac{m^3}{\hbar^3k^3\hbar^3q^3}\,\delta''(\nu-\nu_0). \tag{A.10}$$

The $d\nu$ integration is carried out going through the same steps as in (A.4) and (A.5), this time using the rule

$$f(x)\,\delta''(x) = f(x_0)\,\delta''(x) - 2f'(x_0)\,\delta'(x) + f''(x_0)\,\delta(x). \tag{A.11}$$

The $d(\hbar q)$ integral is lengthy but easy to carry out, and finally the $d(\hbar k)$ integral results essentially in putting $k = k_F$. We obtain

$$\begin{aligned}\alpha_r'' = \frac{Vm^3}{3N\hbar^2\pi}\frac{4\pi V}{(2\pi)^3\hbar^3}\frac{(1+\pi^2x^2)^4}{384\pi(1-A')}(64\pi x)^2\{&-960\pi^2x^2(1+4\pi^2x^2)^4\\ &-72\pi^7x^9(1+\pi^2x^2)^8+384(1+4\pi^2x^2)^4+[\tfrac{27}{64}(x/\pi)-2.625\pi x^3\\ &-12.25\pi^3x^5-7\pi^5x^7](1+\pi^2x^2)^8\}/(1+\pi^2x^2)^8(1+4\pi^2x^2)^4.\end{aligned} \tag{A.12}$$

In the mobility formula (1.1) α_r'' appears in the numerator and α_r' in the denominator, and so to get the zero of μ we have to search where α_r'' goes zero. If we look at the curly bracket term in (A.12) we see that for $x = 0$ it takes the value 384; as x slowly increases it becomes small and passes through zero at $x = 0.201\,290\,399\,297\,936$. After this value of x the curly bracket term always remains negative and does not change sign. There is therefore no root other than $x = 0.2$ in the region $0 \leqslant x \leqslant 1$. The whole expression is very sensitive to changes in the value of x; this is because of the high powers of x appearing in the expression. Practically we may take the root to be $x = 0.2$. Stated in another way this corresponds to $\rho_A^{1/3}a_0 = 0.2$.

References

Debney B T 1976 *J. Phys. C: Solid State Phys.* **9** 3087
Economou E N and Cohen H M 1972 *Phys. Rev.* B **5** 2931
Edwards J T and Thouless D J 1972 *J. Phys. C: Solid State Phys.* **5** 807
Fertis A C, Andriotis A N and Economou E N 1981 *Phys. Rev.* B **24** 5806
Gotze W 1981 *Phil. Mag.* B **43** 219
Ioffe A E and Regel A R 1960 *Prog. Semicond.* **4** 237
Logan D E and Volynes P G 1985 *Phys. Rev.* B **31** 2437
Matsubara T and Toyozawa Y 1961 *Prog. Theor. Phys.* **26** 739
Milinski N 1991 *Prog. Theor. Phys.* **85** 493
Mott N F and Davis E A 1971 *Electronic Processes in Noncrystalline Materials* (Oxford: Oxford University Press)
Unal B 1987 *J. Phys. C: Solid State Phys.* **20** 1765
Unal B and Alkan B 1993 *J. Phys. Soc. Japan* **62** at press
Unal B, Altanhan T and Alkan B 1992 *Prog. Theor. Phys.* **88** 485
Vollhardt D and Wolfle P 1980 *Phys. Rev.* B **22** 4666