

Double Transition Effect in Anderson Transition

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Abstract

In this work we have studied the electronic mobility μ within a completely disordered lattice system by using the strong interatomic hopping potential $V(r) = (-\frac{r}{a_0}) \exp(-r/a_0)$ for site representation of the Hamiltonian. It is shown that a metallic system of a completely disordered lattice first goes insulating and then goes back to metallic again at higher atomic density ρ .

Key Words: Anderson Transition, Double Transition Effect

1. Introduction

Anderson model and Anderson transition concept have played and continue to play important roles in the understanding of disordered systems. The physics of disordered systems is a vast subject with an extensive literature. In three dimensions (3D) it is believed that some of the electronic states are localized, which has important implications on transport coefficients. Intuitively, one expects that if the Fermi level falls into a range of localized states, the conductivity will decrease as the temperature is lowered in contrast to the behavior of pure crystalline material in which it increases due to the freezing out of phonon scattering. On the other hand, if all the states that arise are localized there is the important characteristic behavior of completely disordered conductors where the system goes from a metallic to an insulating state as the disorder is increased. The disorder of the system arises from either lattice irregularity [1] or site-energy randomness [2] or both [3]. In order to examine the transition regime, we first define a disorder parameter wherein by changing this parameter we vary the randomness of the system. So we obtain its value when the system goes from a metallic to an insulating state, which is the so-called Anderson transition. For this purpose there are different methods in literature. For example Debney used the Ioffe-Regel condition $KL=1$, through calculating the mean free path L from first order perturbation theory to find the Anderson transition [4]. Fertis

et al. used the L(E) localization test of Economou and Cohen [5,6], whereas Logan and Volynes used the Fredholm equation technique of Abou-Chacra et al. [7,8]. On the other hand, Vollhard and Wolfe used correlation function technique, directly looking at the transport coefficients [9,10]. In this work we apply the mobility formula of Unal et al. [11]

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

to a completely disordered lattice. Here, e is the electronic charge, N is total number of electrons and α_r', α_r'' are the frequency derivatives of the force-force correlation function $\alpha_r(\omega)$, given by

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

The meaning of each term in this expression will be defined during the evaluation of α_r', α_r'' in the following sections and in Appendix. In this work we consider the density of medium ρ to be the randomness parameter of the system. If we increase the parameter we find that the mobility goes to zero.

2. The Model Hamiltonian

In this paper we study the scattering of electrons in a completely disordered system in which the atomic site positions \vec{R}_i have no regularity [1,4]. At the beginning we assume that the density of the considered system is very low, which means the atoms are far apart from each other. Each atom is assumed to have an effective Bohr radius a_0 and gives a 1s electron to the medium. The mean atomic distance a is given by $a^3 = \frac{\Omega}{N} = \rho^{-1}$, where Ω and N show the volume and the number of atoms, respectively. We assume that the interatomic hopping potential between two sites r distance apart has the form

$$V(r) = -\frac{r}{a_0} e^{-r/a_0}. \quad (3)$$

This expression contains the prefactor r/a_0 besides the exponential term $\exp(-r/a_0)$, and therefore is called the modified exponential interaction. The pure exponential interaction case was studied in ref [12], here we want to see the effect of its modifications on the system properties through employing the potentials $V(r)$ given by Eq. (3). In the quasi-momentum representation the system Hamiltonian $H = H_0 + U$ is given by

$$H_0 = \sum_k H_{kk} C_k^+ C_k \quad (4)$$

$$U = \sum_{k,k'} H_{k,k'} C_{k'}^+ C_k \quad (5)$$

where $H_{k,k'} = \langle k' | H | k \rangle$, $\vec{k}' = \vec{k} + \vec{q}$, and C_k^+, C_k are creation and annihilation operators for the electrons with momentum k ; $\hbar = 1$ units are used throughout. Replacing the diagonal elements of H by their averages, $\langle H_{kk} \rangle = \frac{N}{\Omega} V(k) = -\epsilon(k)$, where $V(k)$ is the Fourier transform of Eq. (3) and $\epsilon(k)$ has the form

$$\epsilon(k) = -\frac{A^3 (3 - a_0^2 k^2)}{8 (1 + a_0^2 k^2)^3}, \quad (6)$$

with $A^3 = 64 (a_0/a)^3 \pi$. The mobility expression given by Eq. (1) contains the terms α'_r, α''_r , and by taking derivatives with respect to frequency ω and then setting $\omega = 0$ we can easily obtain these expressions from Eq. (2) in the form

$$\alpha'_r = \frac{2\pi}{3} \sum_{k,q} \hbar^2 q^2 |U_q|^2 n'_k \delta'(\Delta E') \quad (7)$$

$$\alpha''_r = -\frac{2\pi}{3} \sum_{k,q} \hbar^3 q^2 |U_q|^2 n'_k \delta''(\Delta E'). \quad (8)$$

Here, $\Delta E' = E_{k+q} - E_k$ and n'_k stands for the derivative of occupation number n_k with respect to energy E_k . Later in the calculation of Eqs. (7)-(8) we shall need $|U_q|^2$ showing the departure of the system from its unperturbed state. Making use of Debney's work [4] this is found to be

$$|U_q|^2 = \frac{\epsilon_k^2}{2} + \frac{\epsilon_{k'}^2}{2} + 3 \frac{A^3}{64} + 3A^3 \frac{\left(4 - a_0^2 |\vec{k} + \vec{k}'|^2\right)}{\left(4 + a_0^2 |\vec{k} + \vec{k}'|^2\right)^4}. \quad (9)$$

3. Evaluation of α'_r and α''_r

In order to evaluate the sums in Eqs. (7), (8) we must turn into integrations by using the following relations:

$$\sum_q \rightarrow \frac{V}{(2\pi)^3} \int d^3 q, \quad \sum_k \rightarrow \frac{V}{(2\pi)^3} \int d^3 k, \quad (10)$$

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

$$\Delta E' = -\frac{\hbar^2 k q}{m} \nu + \frac{\hbar^2 q^2}{2m}. \quad (11)$$

Here we assume that there is no meaning of energy wavevector relation in disordered lattices; therefore we have replaced $\Delta E' = E_{k+q} - E_k$ by its parabolic band value using this energy difference, the necessary integrals can be done easily (see Appendix for details). The results α'_r, α''_r are

$$\begin{aligned} \alpha'_r = C_1 & \left[16\pi^3 x^5 \frac{(3 - \pi^2 x^2)^2}{3(1 + \pi^2 x^2)^6} - \frac{16\pi^5 x^7 (3 - \pi^2 x^2)}{3(1 + \pi^2 x^2)^6} \right. \\ & - \frac{16\pi^5 x^7 (3 - \pi^2 x^2)^2}{(1 + \pi^2 x^2)^7} + \frac{\pi^2 x^2}{4} - \frac{3}{16} + \frac{7(1 + \pi^2 x^2)}{24} \\ & + \frac{(1 - \pi^2 x^2)}{6} - \frac{(1 + \pi^2 x^2)^2}{8} - \frac{(1 + \pi^2 x^2)(1 - \pi^2 x^2)}{8} \\ & \left. - \frac{(1 - \pi^2 x^2)}{24(1 + \pi^2 x^2)^3} + \frac{1}{48(1 + \pi^2 x^2)^2} \right], \quad (12) \end{aligned}$$

$$\begin{aligned} \alpha''_r = C_2 & \left[\frac{4096\pi^3 x^5 (3 - \pi^2 x^2)}{(1 + \pi^2 x^2)^6} - \frac{12288\pi^3 x^5 (3 - \pi^2 x^2)^2}{(1 + \pi^2 x^2)^7} \right. \\ & - \frac{2048\pi^5 x^7}{(1 + \pi^2 x^2)^6} - \frac{24576\pi^5 x^7 (3 - \pi^2 x^2)}{(1 + \pi^2 x^2)^7} \\ & \left. - \frac{43008\pi^5 x^7 (3 - \pi^2 x^2)^2}{(1 + \pi^2 x^2)^8} + 24(1 + \pi^2 x^2) - \frac{24(1 - \pi^2 x^2)}{(1 + \pi^2 x^2)^4} \right]. \quad (13) \end{aligned}$$

Here, C_1, C_2 are constants and x is the disorder parameter of the system defined as $x = a_0/a$ and depends on material density by $x = a_0\rho^{1/3}$. If we substitute Eqs. (12),(13) into Eq. (1) we obtain the mobility expression μ as a function of x . As mentioned at the beginning, we have considered first a system whose density is very low. In this case the mean interatomic distance a is large, corresponding to small value of x . In other words the atoms in the system are far apart from each other and we expect that the probability of the scattering of an electron should be small. The mobility will then have a large value. If we increase the disorder parameter, x , corresponding to the small distances between the atoms, the scattering of an electron with atoms will take place more effectively. So, the value of mobility will start falling during the process. If we go on changing the

randomness parameter x still further, we normally expect the value of α_r'' to become zero at some point x_c and hence μ to become zero also. While carrying these changes we should observe that α_r' never goes to zero, because it stays in the denominator of Eq. (1). Indeed our α_r' satisfies this requirement and gives no root as a function of x . In Fig. 1 we have drawn α_r'' against x , but this time it has given double transition effect, first going to insulating phase at $x_{c1} = 0.23$ and then at $x_{c2} = 0.34$ going back to metallic case again and remaining so at higher densities. This unusual behavior will be explained in the next section in terms of the potential $V(r)$.

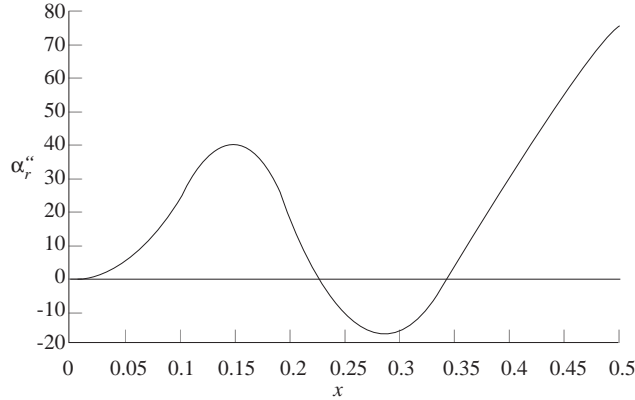


Figure 1. Behavior of α_r'' as a function of x

4. Conclusion

As we mentioned in the introduction, Anderson transition changes markedly the transport properties of condensed matter, therefore this effect may be taken up via studying transport coefficients. There are different methods and techniques for calculating these coefficients. One of them has been developed by Unal et al. [11] is and given by Eq. (1), which depends on the correlation function technique [9,10]. This formula was applied to a dilute system with pure exponential interactions before, and a result of about $x_c = 0.31$ [12] is obtained for the ones existing in literature for the Anderson transition. In this paper we applied it to the completely disordered structure with a modified exponential interaction of the type given by Eq. (3) to see effect of changing the potential parameters. The hopping potential presently at hand differs from the previously considered ones in that it becomes zero in the limit of small interatomic distance $r \rightarrow 0$. This is due to the fact that r appears as multiplied by the exponential e^{-r/a_0} . Now if we choose a pair of atoms, one being fixed, completely disordered lattice model requires that the other atom can be found anywhere inside the system including the position of the first atom, this allows r to be zero. Considering different configurations of our system, this second atom may be viewed as moving around the fixed one. When the atomic density is low, the moving atom prefers mainly the large distances r , $V(r)$ is then small so its scatter-

ing effect is sufficiently weak to make the system metallic. For high atomic densities on the other hand, small values of r becomes highly probable, $V(r)$ is again small and its scattering effect is also small, hence in this limit too the system should be metallic. The above mentioned behavior of potential $V(r)$ explain why the system cannot stay in the insulating phase forever after the first transition at x_{c1} as the density is increased. In the pure exponential case [12] the system remained insulating once a transition had taken place at x_c , because that potential did not behave as the present one for higher density. In this work we have shown that double transition effect may occur in certain interatomic hopping potentials which is a new result within the Anderson transition concept.

Appendix

In order to calculate α'_r , first of all we put the expressions $|U_q|^2$ and $\Delta E'$ given by Eqs. (9) and (11) into Eq. (7). We have

$$\alpha'_r = \frac{2\pi}{3} \sum_{k,q} \hbar^2 q^2 \left[\frac{\epsilon_k^2}{2} + \frac{\epsilon_{k'}^2}{2} + \frac{3}{64} A^3 + 3A^3 \frac{[4 - a_0^2 (4k^2 + q^2 - 2kq\nu)]}{[4 + a_0^2 (4k^2 + q^2 - 2kq\nu)]^4} \right] \cdot \left[1 - \left(\frac{dA}{d\epsilon_k} \right) \right]^{-1} \delta(\epsilon_f - \epsilon_k) \delta' \left(-\frac{\hbar k \hbar q}{m} \nu + \frac{\hbar^2 q^2}{2m} \right) \quad (\text{A.1})$$

for the n'_k we have used the result taken from Ref. [13]. In the calculation of α_r we write it in the form $\alpha'_r = \alpha'_{r1} + \alpha'_{r2} + \alpha'_{r3} + \alpha'_{r4}$. Each term is given by the following:

$$\alpha'_{r1} = \frac{2\pi}{3} \frac{1}{1-A'} \frac{1}{2} \sum_{k,q} \hbar^2 q^2 \epsilon_k^2 \cdot \delta(\epsilon_f - \epsilon_k) \delta' \left(-\frac{\hbar k \hbar q}{m} \nu + \frac{\hbar^2 q^2}{2m} \right) \quad (\text{A.2})$$

$$\alpha'_{r2} = \frac{2\pi}{3} \frac{1}{1-A'} \frac{1}{2} \sum_{k,q} \hbar^2 q^2 \epsilon_{k'}^2 \cdot \delta(\epsilon_f - \epsilon_k) \delta' \left(-\frac{\hbar k \hbar q}{m} \nu + \frac{\hbar^2 q^2}{2m} \right) \quad (\text{A.3})$$

$$\alpha'_{r3} = \frac{2\pi}{3} \frac{3A^3}{64} \frac{1}{1-A'} \frac{8 \left(1 + a_0^2 k_f^2 \right)^4}{A^3 \left(-20a_0^2 k_f + 4a_0^2 k_f a_0^2 k_f^2 \right)} \cdot \sum_{k,q} \hbar^2 q^2 \delta(\hbar k - \hbar k_f) \delta' \left(-\frac{\hbar k \hbar q}{m} \nu + \frac{\hbar^2 q^2}{2m} \right) \quad (\text{A.4})$$

$$\alpha'_{r4} = \frac{2\pi}{3} \frac{3A^3}{1-A'} \frac{8(1+a_0^2 k_f^2)^4}{A^3(-20a_0^2 k_f + 4a_0^2 k_f a_0^2 k_f^2)} \cdot \sum_{k,q} \hbar^2 q^2 \delta(\hbar k - \hbar k_f) \delta' \left(-\frac{\hbar k \hbar q}{m} \nu + \frac{\hbar^2 q^2}{2m} \right) \quad (\text{A.5})$$

To evaluate the above Eqs. (A.2), (A.3), (A.4) and (A.5), first the sums over \vec{q} are turned into integrals in the usual way and for integration over $d\nu$ we use the property

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

with $\nu_0 = \frac{\hbar q}{2\hbar k}$. For the calculation of the $d(\hbar q)$ integration we employ the technique used in Ref. (11). Finally, $d^3(\hbar k)$ integration is carried out to obtain

$$\alpha'_r = C_1 \left[16\pi^3 x^5 \frac{(3 - \pi^2 x^2)^2}{3(1 + \pi^2 x^2)^6} - \frac{16\pi^5 x^7 (3 - \pi^2 x^2)}{3(1 + \pi^2 x^2)^6} - \frac{16\pi^5 x^7 (3 - \pi^2 x^2)^2}{(1 + \pi^2 x^2)^7} + \frac{\pi^2 x^2}{4} - \frac{3}{16} + \frac{7(1 + \pi^2 x^2)}{24} + \frac{(1 - \pi^2 x^2)}{6} - \frac{(1 + \pi^2 x^2)^2}{8} - \frac{(1 + \pi^2 x^2)(1 - \pi^2 x^2)}{8} - \frac{(1 - \pi^2 x^2)}{24(1 + \pi^2 x^2)^3} + \frac{1}{48(1 + \pi^2 x^2)^2} \right]. \quad (\text{A.6})$$

Evaluation of α''_r is carried out in a similar way.

References

- [1] T. Matsubara and Y. Toyozawa, *Prog. Theor. Phys.*, **26** (1961) 739.
- [2] J.T. Edwards and D.J. Thouless, *J. Phys. C: Solid State Phys.*, **5** (1972) 807.
- [3] N.F. Mott and E.A. Davis, *Electronic Processes in Non-crystalline Materials* (Oxford: Oxford University Press) 1971.
- [4] B.T. Debney, *J. Phys. C: Solid State Phys.*, **9** (1976) 3087.
- [5] E.N. Economou and H.M. Cohen, *Phys. Rev.*, **B5** (1972) 2931.

- [6] A.C. Fertis, A.N. Andriotis and E.N. Economou, *Phys. Rev.*, **B24** (1981) 5806.
- [7] D.E. Logan and P.G. Volynes, *Phys. Rev.*, **B31** (1985) 2937
- [8] R. Abou-Chacra, P.V. Anderson and D.J. Thouless, *J. Phys. C: Solid State Phys.*, **6** (1973) 1734.
- [9] D. Vollhardt and P. Wölfle, *Phys. Rev.*, **B22** (1980) 4666.
- [10] W. Götze, *Phil. Mag.*, **B43** (1981) 219.
- [11] B. Ünal, T. Altanhan and B. Alkan, *Prog. Theor. Phys.*, **88** (1992) 485.
- [12] B. Alkan and B. Ünal, *Il Nuovo Cim.*, **17D N.2** (1995) 209.
- [13] B. Ünal, *J.Phys. C: Solid State Phys.*, **20** (1987) 176.