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Electronic conduction through quantum dots undergoing Jahn–Teller transition

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ABSTRACT

Electronic conduction through quantum dots undergoing Jahn–Teller distortion is studied utilizing a model presented recently in connection with investigation of possible magnetovoltaic effect in this system. The quantum dot connected to two metallic leads is described by the single impurity Anderson model (SIAM) Hamiltonian along with two additional terms describing the Jahn–Teller distortion and an applied magnetic field. The self-consistent calculation shows that the Jahn–Teller (J–T) order parameter which is a measure of the splitting of the degenerate dot level is maximum at zero temperature and smoothly goes to zero at the structural transition temperature, T_s. The conductance is greatly suppressed by the J–T distortion at low temperatures, slowly increases and attains a maximum at T_s, above which it shows a slow decrease. When plotted as a function of the energy of the dot level, the conductance shows two peaks corresponding to the two split J–T levels at temperatures below T_s, which further develops into a four peak structure in the presence of a magnetic field.

1. Introduction

A quantum dot, being an agglomeration of a small number of atoms, behaves like a large atom with quantized energy levels with confined electrons [1,2]. If one attaches metallic leads to the two ends of the quantum dot and applies a voltage across it, the electrons from the conduction band of the lead can tunnel through the barrier at the boundary and get into the localized level of the dot and tunnel to the other lead, resulting in an electronic transport across the quantum dot.

The experimental study of the conductance through a quantum dot has revealed many interesting features [3–5]. For these experiments the quantum dots were fabricated by putting suitable metallic gates in the inversion layer of Silicon [3] and in GaAs heterostructures [4] so as to create a narrow channel in a two dimensional electron gas. The measured conductance showed periodic oscillations with applied gate voltage in both the experiments. The attempts to interpret these oscillations resulted in attributing them to the presence of pinned charge density waves (CDW) in the one dimensional electron channel in the Si inversion layer [3] and the transport to the sliding of the pinned CDW every time a single electron is added to the channel. In the measurement of the GaAs heterostructure the authors were able to correlate the period of the oscillations with the length of the narrow channel.

Electronic conduction in a quantum dot can be described in terms of the single impurity Anderson model (SIAM) [6]; originally proposed in the context of the study of the appearance of a magnetic moment when a transition metal impurity atom is placed in a nonmagnetic host metal. This model was adapted to the problem of electrical transport in a quantum dot [5] connected to metallic leads. The quantum dot is characterized by its localized levels due to confinement. Each of these levels when doubly occupied by the electrons, will result in the strong on-site Coulomb repulsion between them. The Fermi sea of the electrons in the left and right metallic leads which are assumed to be ideal, replaces the free electrons of the host metal in the original Anderson model. These electrons can tunnel through the barriers into the localized dot level because of the hybridization of the quantum dot level and the lead states.

Recently there has been a lot of interest in the study of quantum dots with a magnetic impurity [7–14] because of the recent surge of interest in the phenomenon of 'Spintronics' or spin

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electronics. In order to deal with this problem, the Anderson model has been further generalized to include an additional interaction term in the Hamiltonian describing the coupling of the spin of the dot electrons with the impurity spin in the form of an exchange (s–d) interaction [14].

An experimental realization of the fact that a quantum dot essentially consists of a cluster of atoms to which metallic leads can be attached was reported in Ref. [11] in the context of studying the Kondo effect in a gold quantum dot by embedding magnetic impurities in the metallic leads. It is well known that a small cluster of atoms could have many isomeric structures [15] differing in energy only by a small amount, hence becoming susceptible to the possibility of undergoing structural transformations. A possible electronic mechanism by which such a structural change can be brought about in a quantum dot could be through the Jahn–Teller effect, if the ground state of the dot happens to be degenerate. If the gain in electronic energy can overcome the cost in elastic energy due to the lattice distortion, then the structural phase transition will be stabilized below a critical temperature T_s and the levels will split.

In a recent publication [16] we extended the Anderson model to study the effect of the interplay between the Coulomb potential and an applied magnetic field in a quantum dot capable of undergoing Jahn–Teller distortion and showed that under suitable conditions this interplay may lead to the production of an oscillatory voltage which we called the magnetovoltaic effect.

In this paper we use the same model to study the effect of Jahn–Teller distortion and the role of magnetic field on the electrical conductance of a quantum dot capable of undergoing a structural phase transition. Results of this study have been reported in recent conference proceedings [17,18].

In Section 2 the Hamiltonian for the quantum dot undergoing structural transition with two metallic leads attached to it is first set up. We then calculate the Green's function for the electrons in the quantum dot by using the equation of motion technique [19]. This Green's function is then used in the Landauer type formula to obtain conductance through the quantum dot [20,21]. Results of our calculation are presented in Section 3. The final conclusions of the paper are drawn in Section 4.

2. Theory

We have modeled our quantum dot connected to two ideal metal leads, by the single impurity Anderson model (SIAM) Hamiltonian [6] together with two additional terms representing the structural transition due to Jahn–Teller distortion, and the external magnetic field. The localized levels of the quantum dot correspond to the electronic levels of the impurity atom, and the Fermi sea of the electrons in the left and right metallic leads represents the free electrons of the host metal in the original Anderson model. These electrons can tunnel through the barriers into the localized dot level because of the hybridization of the two [5]. The dot level being degenerated may be possible to avoid their double occupancy by electrons and hence the Coulomb potential when two electrons tunnel from the lead into the dot. Therefore, a mean field treatment of the onsite Coulomb repulsion term in the dot Hamiltonian may be justified as a first approximation. The Hamiltonian of the system is written in the mean field approximation as

$$H_T^{MF} = \sum_{\alpha,k\sigma}^{L,R} \varepsilon_{\alpha k\sigma} c_{\alpha k\sigma}^{\dagger} c_{\alpha k\sigma} + \sum_{i\sigma}^{1,2} \varepsilon_{i\sigma} n_{i\sigma} + \sum_{i\alpha,k\sigma}^{1,2;L,R} V_{\alpha i}(c_{\alpha k\sigma}^{\dagger} d_{i\sigma} + d_{i\sigma}^{\dagger} c_{\alpha k\sigma}) \quad (1)$$

The first term on the right hand side describes the electrons in the left and the right leads, the second term contains contributions from the electronic states of the quantum dot in the mean field approximation, the applied magnetic field, and the Jahn–Teller distortion. The third term represents the hybridization between the lead electrons and the dot electrons. In this equation $\alpha = L, R$ stands for the left and right leads, $\varepsilon_{\alpha k\sigma}$ the energy of the electron in the α-th lead having wave vector k and spin σ, and $c_{\alpha k\sigma}(c_{\alpha k\sigma}^{\dagger})$ are the annihilation (creation) operators for these electrons. The index $i=1,2$ represents the two degenerate levels of the quantum dot where $\varepsilon_{i\sigma}$ is the effective energy of the localized level and $d_{i\sigma}(d_{i\sigma}^{\dagger})$ the annihilation (creation) operator for the dot electron in the i-th level with spin σ, and $n_{i\sigma} = d_{i\sigma}^{\dagger} d_{i\sigma}$ is the number operator for the dot electrons at the level i with spin σ. The hybridization matrix element is $V_{\alpha i}$. In Eq. (1) the spin dependent energies of the dot levels are given by

$$\varepsilon_{i\sigma} = (\varepsilon_i + U\langle n_{i-\sigma}\rangle - z_\sigma h) \quad (2)$$

where $\varepsilon_{i=1,2} = (\varepsilon_d \pm \Delta_{JT})$ are the two split degenerate levels with a Jahn–Teller splitting of $2\Delta_{JT}$. The second term on the right hand side of this equation is the intra-site Coulomb repulsion between the dot electrons treated in the mean field approximation, U being the intra-level Coulomb repulsion parameter. The third term in Eq. (2) is the contribution from the magnetic field where h is the magnetic field energy and for $\sigma = \uparrow(\downarrow)$ we have the corresponding values $z_\sigma = \pm 1$. Note that Eq. (1) has a simple form involving only quadratic terms in the annihilation (creation) operators which can be solved exactly.

The Jahn–Teller order parameter Δ_{JT} can be calculated from

$$\Delta_{JT} = -\mathcal{G}(\langle n_{1\uparrow}\rangle + \langle n_{1\downarrow}\rangle - \langle n_{2\uparrow}\rangle - \langle n_{2\downarrow}\rangle), \quad (3)$$

where $\mathcal{G}$ is the renormalized electron–phonon coupling constant.

The calculation of the average value of the number operator with spin σ, i.e. $\langle n_{i\sigma}\rangle$ appearing in the above equations involves the spectral density function which is given by the imaginary part of the retarded single particle Green's function for the electrons in the quantum dot. This Green's function has been calculated for this Hamiltonian by using the equation of motion method of the double time Green's function [19] and has been found to be

$$G_{i\sigma,i\sigma}(\omega) = \frac{1}{2\pi[\omega - \varepsilon_{i\sigma} - i\gamma_i]}, \quad (4)$$

where γ_i represents the coupling of the two dot levels to the electrons in the leads and is related to $V_{\alpha i}^2$ via the density of states of electrons ($\gamma_{\alpha i} = \pi |V_{\alpha i}^2| \rho(\omega)$) in the leads.

The average value of the number operator with spin σ, i.e. $\langle n_{i\sigma}\rangle$ can be expressed in terms of this Green's function as

$$\langle n_{i\sigma}\rangle = \int_{-\infty}^{+\infty} d\omega f(\omega) 2\,\mathrm{Im}\, G_{i\sigma,i\sigma}(\omega) = \frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega f(\omega) \frac{\gamma_i}{[(\omega - \varepsilon_{i\sigma})^2 + \gamma_i^2]} \quad (5)$$

where $f(\omega)$ is the Fermi distribution function.

We have also calculated the conductance for the system by using the Landauer type formula [20,21]

$$G = \frac{2e^2}{h}\sum_{i\sigma}\gamma_i \int_{-\infty}^{+\infty} d\omega \left(-\frac{df(\omega)}{d\omega}\right) \mathrm{Im}\, G_{i\sigma,i\sigma}(\omega) = \left(\frac{2e^2}{h}\right)\sum_{i\sigma}\gamma_i^2 \int_{-\infty}^{+\infty} d\omega(-f'(\omega)) \times \left\{\frac{1}{[(\omega - \varepsilon_{i\sigma})^2 + \gamma_i^2]}\right\} \quad (6)$$

Recalling the definition of $\varepsilon_{i\sigma}$ as given by Eq. (2) it is evident that the average $\langle n_{i\sigma}\rangle$ depends on the average occupation of the level i by electrons with spin $-\sigma$ i.e., $\langle n_{i-\sigma}\rangle$ and vice versa. Hence