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Conductance through a single nonlinear impurity

M.I. Molina [a,*], H. Bahlouli [b]

[a] *Facultad de Ciencias, Departamento de Física, Universidad de Chile, Casilla 653, Santiago 21, Chile*
[b] *Department of Physics, KFUPM, Dhahran 31261, Saudi Arabia*

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Abstract

We use the discrete nonlinear Schrödinger (DNLS) equation to describe tunneling through a single magnetic impurity connected to two perfect leads, in the presence of a magnetic field. Due to the presence of a strong on-site nonlinear interaction between two opposite spins at the impurity site, the zero voltage conductance exhibits strong correlations between parallel and anti-parallel spin conduction channels. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Nonlinear effects have been the subject of intense research in condensed matter physics, both from the theoretical and experimental point of view [1]. This is due, in part, to the wide range of potential applications in the design of new optical and electronic devices for computing and communications. For instance, it has been shown that nonlinearity gives rise to multistability, noise and might originate a chaotic behavior in certain systems. Transport properties of nonlinear chains of atoms and double barrier structures under applied electric fields have been recently examined by Cota et al. [2]. Their work shows that resonances shift in the presence of nonlinearity and that their width decreases as the nonlinearity becomes stronger. A subclass of nonlinear problems that also have received attention recently is the problem of single, or few, nonlinear impurities embedded in a linear host [3–6]. In these cases, the source of the nonlinearity is a strong coupling between an excitation and a local vibrational mode. In the approximation where one assumes a rapid readjustment of the local vibration to the presence of the excitation, one quickly arrives at the discrete nonlinear Schrödinger (DNLS) equation as the effective evolution equation for the excitation [7]. By using an extension of the Green's function formalism, it has been possible to examine the formation of bound states in one-dimensional [3], two-dimensional [5] and three-dimensional lattices [6].

Nonlinearity is also relevant to transport problems in nanoscale devices [8]: It is known that the electron–electron interaction is important in any serious study of the transport properties of small systems such as quantum

* Corresponding author.
E-mail addresses: mmolina@abello.dic.uchile.cl (M.I. Molina), bahlouli@kfupm.edu.sa (H. Bahlouli).

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dots and few impurity models [9]. Generally speaking, the Coulomb interaction gives rise to a nonlinear term in the Schrödinger equation. In this case the Coulomb interaction is modeled by a cubic, nonlocal term in the equation of motion of the corresponding fermionic field operators. To proceed further a Hartree–Fock approximation for the nonlinear term is used [10]. One can also use a perturbative approach in the Coulomb interaction [11].

In this Letter we take the alternative approach of modelling the effect of the electron–electron interaction by a nonlinear local term in the Schrödinger equation. One can look at such an approximation as being a Hartree-like approximation of the original many-body problem. We examine a one-dimensional nonlinear impurity problem where the source of the nonlinearity is due to the presence of a strong on-site Coulomb interaction between the two opposite spins at the impurity site, rather than to a strong electron–phonon coupling. Since the spin degree of freedom plays an important role in the correlated transport through the localized impurity state, a study of the magnetic field dependence of the linear conductance will exhibit a lift of the degeneracy of the two spin states when a strong magnetic field is applied. That is why we will focus on the zero voltage conductance as a function of the external magnetic field.

2. Theoretical model

We consider the problem of the transmission of an electron incident with energy E, upon a strongly localized impurity region where electron–electron interaction is important. In the impurity region we impose a strong local interaction term that mimics the on-site Coulomb interaction $U\rho_{0\sigma}\rho_{0-\sigma}$ which is proportional to both spin up and spin down local densities, $\rho_{0\sigma} = |\Psi_{0\sigma}|^2$, where $\Psi_{0\sigma}$ is the probability amplitude of finding an electron at the impurity site. U is a parameter measuring the strength of the local Coulomb interaction. This repulsive interaction arises from the charge accumulation and shifts the energy levels of the opposite spin states. Thus we expect our model to adequately describe the nonlinear effects due to charge accumulation at the impurity site, and will also be valid in the extreme case of a quantum dot containing only one level.

The model consists of three regions: a single magnetic impurity at $n = 0$, and two perfect semi-infinite leads on the left $-\infty < n < 0$ and the right $0 < n < +\infty$ described by a tight binding Hamiltonian. The noninteracting electrons in the leads are described by

$$H_0 = \sum_{n,\sigma}\left[\epsilon_{n,\sigma}\Psi^*_{n,\sigma}\Psi_{n,\sigma} + \sum_{m\neq n} V_{n,m}\Psi^*_{n,\sigma}\Psi_{m,\sigma}\right], \tag{1}$$

where $\Psi_{n,\sigma}(t)$ and $\epsilon_{n,\sigma}$ are the probability amplitude of finding the electron at site n and the corresponding local energy, respectively, at site n for an electron with spin σ. The on site energy $\epsilon_{n,\sigma} = \epsilon_n - \sigma B$ is defined in terms of the zero-field on-site energy level ϵ_n shifted by the Zeeman energy. $V_{n,m}$ is the overlap integral which, in general, depends only on the distance between the two sites m and n, so that $V_{n,m} = V_{m,n}$. The localized impurity state is described by

$$H_I = \sum_{\sigma}\left[\epsilon_{0,\sigma}\Psi^*_{0,\sigma}\Psi_{0,\sigma} + \frac{1}{2}U|\Psi_{0,\sigma}|^2|\Psi_{0,-\sigma}|^2\right]. \tag{2}$$

U is the strength of the on-site interaction and $\epsilon_{0,\sigma}$ is the local energy at the impurity site. Putting these Hamiltonians together and including the hopping between the leads and the impurity localized state (which we will denote later as V_L and V_R for the left and right leads), we obtain the total Hamiltonian:

$$H = \sum_{n,\sigma}\left[\epsilon_{n,\sigma}\Psi^*_{n,\sigma}\Psi_{n,\sigma} + \sum_{m\neq n} V_{n,m}\Psi^*_{n,\sigma}\Psi_{m,\sigma} + \frac{1}{2}U\delta_{n,0}|\Psi_{n,\sigma}|^2|\Psi_{n,-\sigma}|^2\right]. \tag{3}$$

It is clear from our model Hamiltonian that the nonlinear interaction exists only at the impurity site $n = 0$, and its magnitude is proportional to the product of the probability densities of up and down spin states at the impurity site. From this point of view this interaction term mimics the famous Hubbard term $Un_{\uparrow}n_{\downarrow}$ in the Hamiltonian formalism. Besides this apparent similarity there is no connection between our model which deals with an approximate nonlinear equation for the probability amplitudes and the actual Hubbard Hamiltonian which deals with fermionic field operators.

The field amplitudes $\Psi_{n,\sigma}$ and $i\Psi^*_{n,\sigma}$ form canonically conjugate variables and $i\ (d/dt)\Psi_{n,\sigma} = -\partial H/\partial\Psi^*_{n,\sigma}$ is the corresponding equation of motion. From the above Hamiltonian we then obtain

$$i\frac{d}{dt}\Psi_{n,\sigma} + \sum_m V_{n,m}\Psi_{m,\sigma} + \left(\epsilon_{n,\sigma} + U\delta_{n,0}|\Psi_{n,-\sigma}|^2\right)\Psi_{n,\sigma} = 0. \tag{4}$$

This equation is a variant of the discrete nonlinear Schrödinger (DNLS) equation whose properties been studied extensively in recent years. It is worth mentioning that the DNLS equation can be derived, in principle, from the more general nonlinear Schrödinger equation $i\partial_t\Psi + \partial_x^2\Psi + f(x,|\Psi|^2)\Psi = 0$. The function $f(x,|\Psi|^2)$ characterizes the nonlinearity of the interaction, e.g., self-interaction of the quasiparticles in the system. The complete integrability of this equation for $f(x,|\Psi|^2) = |\Psi|^2$ was established in a seminal paper by Zakharov and Shabat [12]. The origin of the nonlinearity in our case stems from the local Coulomb interaction and shifts the energy levels of opposite spins at the impurity site. However, the local nature of this interaction term makes it inadequate to describe the long range Coulomb interaction. Thus, our model (4) does not correspond to the well-known Hubbard model, often used as a model Hamiltonian to describe nanostructure devices. Also, Eq. (4) does not even correspond to the classical Hartree approximation of the Hubbard model. In the Hartree approximation, the nonlinear term is described not by a single orbit as described in Eq. (4) but rather by the sum of all orbits below the Fermi level. Nevertheless, the discrete nonlinear Schrödinger (DNLS) equation (4) does contain some essential features of the interacting system, such as the repulsive and nonlinear nature of the interaction.

Let us find the stationary states of (4), i.e., we look for solutions of the type $\Psi_{n,\sigma}(t) = e^{iEt}\Psi_{n,\sigma}(E)$, where E is the associated eigenvalue. We restrict ourselves to a nearest-neighbors tight-binding approximation. Let $V_{n,n+1}$ be the hopping integral between the nth and the $(n+1)$th site, then under these assumptions our previous equation becomes

$$(E - \epsilon_{n,\sigma})\Psi_{n,\sigma} = V_{n,n-1}\Psi_{n-1,\sigma} + V_{n,n+1}\Psi_{n+1,\sigma} + \delta_{n,0}U|\Psi_{n,-\sigma}|^2\Psi_{n,\sigma}. \tag{5}$$

We now choose the hopping integrals as follows:

$$V_{n,n+1} = \begin{cases} V_L & \text{for } n = -1, \\ V_R & \text{for } n = 0, \\ V & \text{for } n \neq -1, 0. \end{cases} \tag{6}$$

That is, the hopping within the leads is V while the links of the magnetic impurity with the left and right leads are V_L and V_R, respectively. The latter express the degree of hybridization of the localized impurity state with the extended states at the leads. For $n = -1$, 0 and 1, the eigenvalue equation (5) reads

$$(E - \epsilon_{0,\sigma})\Psi_{0,\sigma} = V_L\Psi_{-1,\sigma} + V_R\Psi_{1,\sigma} + U|\Psi_{0,-\sigma}|^2\Psi_{0,\sigma}, \tag{7}$$

$$(E - \epsilon_{-1,\sigma})\Psi_{-1,\sigma} = V\Psi_{-2,\sigma} + V_L\Psi_{0,\sigma}, \tag{8}$$

$$(E - \epsilon_{1,\sigma})\Psi_{1\sigma} = V_R\Psi_{0,\sigma} + V\Psi_{2,\sigma}. \tag{9}$$

To study the scattering properties of our single magnetic impurity located at the origin, we send a plane wave towards $n = 0$ from the left and study its transmission. Thus, we assume a solution of the form

$$\Psi_{n,\sigma} = \begin{cases} (I_\sigma e^{ikn} + R_\sigma e^{-ikn})\chi_\sigma & \text{for } n \leqslant -1, \\ T_\sigma e^{ikn}\chi_\sigma & \text{for } n \geqslant 1. \end{cases} \tag{10}$$

Here, χ_σ describes the electronic spin state which is assumed to be conserved all along the transmission process since we are ignoring spin flip processes.

After inserting Eq. (10) into Eqs. (7)–(9), and after using the lead's dispersion relation $E = 2V\cos(k)$, where the on-site energy is set to zero for simplicity, the transmission coefficient $\tau_\sigma \equiv |T_\sigma|^2/|I_\sigma|^2$ is found to obey the following nonlinear equation:

$$\tau_\sigma = \frac{4V_L^2 \sin^2 k}{|(V/V_R)(2V\cos(k) - \epsilon_{0,\sigma} - U(V/V_R)^2 \tau_{-\sigma}|I_{-\sigma}|^2) - V_R(1+(V_L/V_R)^2)e^{ik}|^2}. \tag{11}$$

We note that the initial wave amplitude $|I_{-\sigma}|$ renormalizes the nonlinearity term to an effective Coulomb strength $U_{\text{eff}} = U|I_{-\sigma}|^2$. Since we are interested in spin effects rather than in renormalization effects due to the incident wave, we set the amplitude of the incident wave to unity independently of the spin, $|I_\sigma|^2 = |I_{-\sigma}|^2 = 1$. This simplifying assumption will not affect the conclusions of our present work. Our previous equation for τ_σ can be rendered in the compact form

$$\tau_\sigma = \frac{D}{C_\sigma + B_\sigma \tau_{-\sigma} + A\tau_{-\sigma}^2}, \tag{12}$$

where

$$A = \left(\frac{V}{V_R}\right)^6 U^2,$$

$$B_\sigma = 2U\left(\frac{V}{V_R}\right)^2\left[-\left(\frac{V}{V_R}\right)^2\bigl(2V\cos(k) - \epsilon_{0,\sigma}\bigr) + V\left(1 + \frac{V_L^2}{V_R^2}\right)\cos(k)\right],$$

$$C_\sigma = \frac{V^2}{V_R^2}\bigl[2V\cos(k) - \epsilon_{0,\sigma}\bigr]^2 + V_R^2\left(1 + \frac{V_L^2}{V_R^2}\right)^2 - 2V\bigl[2V\cos(k) - \epsilon_{0,\sigma}\bigr]\left(1 + \frac{V_L^2}{V_R^2}\right)\cos(k),$$

$$D = 4V_L^2 \sin^2(k).$$

3. Transmission features

The solution of the above equation for τ_σ seems quite demanding at first sight. Not only do we have a nonlinear transmission, but the spins are also correlated due to the fact that transmission for the up spin depends on the transmission of the down spin, as it is clear from Eq. (12). The transmission formula reduces to the spinless case of Tsironis et al. [4] when we set $V_L = V_R = V$ and $B = 0$. Eqs. (12) can be combined into an algebraic fifth-order equation for τ_σ, which we solve numerically. Hereafter, we assume $V_L = V_R = V$ for simplicity. That is, if we assume that our problem represents an impurity within a barrier, then the equality of the left and right hopping matrix elements amounts to have the impurity at the center of the barrier. In all our numerical computations we set the energy unit to be the host hopping integral (i.e., $V = 1$) and all other energies are counted in units of V. Fig. 1 shows some plots of τ_σ versus $\cos(k)$, for a fixed value of U ($U/V = 3$) and several magnetic field intensities. In general, the transmission for spin up (parallel to the magnetic field) is different from the one for spin down (anti-parallel to the magnetic field), in the presence of a nonzero B. Starting from zero field, the transmissivity for up spins seems to increase with B, reaches a maximum (where resonances occur) and then decreases upon further increment in B. The fact that the magnetic field lowers the energy of the up spins and increases the energy of the down spins plays an important role in the transport properties of the spin channel. In our case since we set all site energies to zero (i.e., $\epsilon_n = 0$) we end up with $\epsilon_{0\sigma} = -\sigma B$, $\sigma = \pm$. Thus the application of a magnetic field transforms our impurity site either to an effective potential well ($\epsilon_{0\uparrow} = -B$) or potential barrier ($\epsilon_{0\downarrow} = B$). The transmission, on the other hand, is enhanced for potential wells while it is suppressed for potential barriers as it is clearly exhibited in Fig. 1. Due to our particular choice of parameters, $V_L = V_R = V = 1$, the magnetic impurity is strongly coupled to the leads and this results in a broad transmission curve as it is observed in this figure.

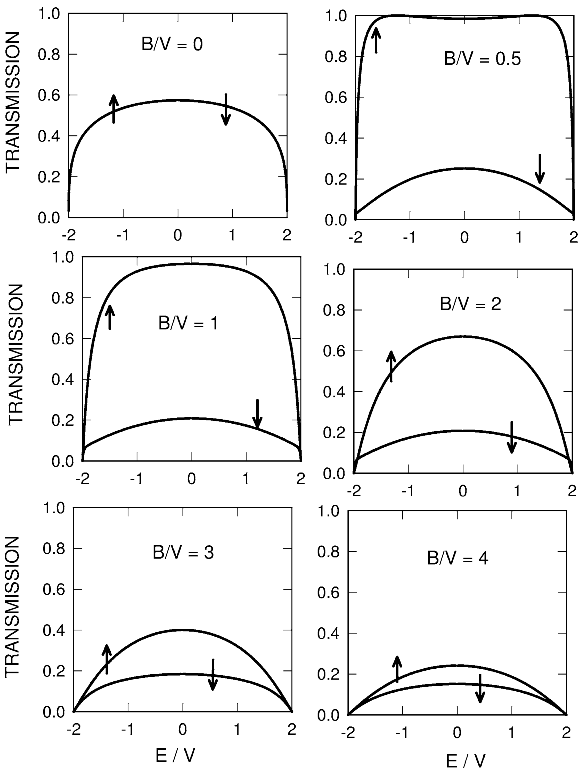

Fig. 1. Transmission coefficient across the magnetic impurity for both channels, parallel (up) and antiparallel (down) to the external field, as a function of the incoming plane wave energy, for different values of the external field B ($U = 3$, $V_L = V_R = V = 1$).

A simple analysis from Eq. (12) shows that at resonance ($\tau_\sigma = 1$), the plane wave energy satisfies

$$\cos^2(k) = 1 - \frac{(\sigma B/V^2)(\sigma B + U)^2}{U - \sigma B}.$$

And, since $0 \leqslant \cos^2(k) \leqslant 1$, we deduce that a resonance is only possible when $\sigma B > 0$ (i.e., $\sigma = +$ or parallel spin) and $U > \sigma B$. Also, it is possible to show that the maximum σB value at which a resonance occurs is $1/\sqrt{2}$ when $U/V = 3/\sqrt{2}$. Fig. 2 shows the resonant energies in terms of B, for several U values. As anticipated, the curves never extend beyond $B/V = 1/\sqrt{2}$. As U/V is increased past $3/\sqrt{2}$, the curves begin to contract towards the $B = 0$ axis.

In the limit of large U (keeping B fixed), important for Coulomb correlations effects, it can be shown that the transmission for both spin signs approach a common limit:

$$\tau_\sigma \to \frac{1 - \cos(2k)}{(B/V)^2 + 2(1 - \cos(2k))}.$$

Similarly, for B large, keeping U fixed, the transmission for both spins approach

$$\tau_\sigma \to \frac{4V^2(1 - \cos(2k))}{B^2}.$$

We therefore conclude that, regardless of the value of the Coulomb energy U, the presence of a strong external magnetic field will decrease the transmission as $1/B^2$.

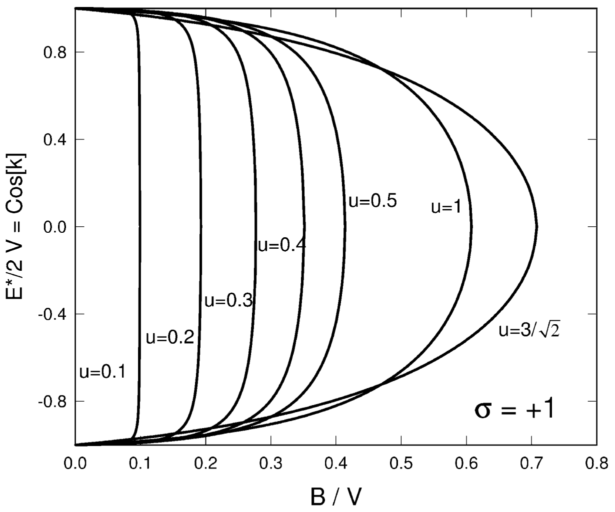

Fig. 2. Resonant energies E^* as a function of the external field B, for different normalized Coulomb correlation energies $u \equiv U/V$. The curves never extend beyond $B/V = 1/\sqrt{2}$ which occurs at $u = 3/\sqrt{2}$.

4. Coulomb interaction effect on the conductance

In order to obtain a realistic picture of our model, it is necessary to include in our study finite temperature effects. The two-probe conductance (in units of $2e^2/\hbar$) at finite temperature is defined by the thermal average of the transmission coefficient [13]:

$$G(T,\mu) = \sum_{\sigma} \int \left(-\frac{\partial f(\mu, E)}{\partial E} \right) \left| \tau_\sigma(E) \right|^2. \tag{13}$$

Here $f(\mu, E)$ is the Fermi–Dirac distribution function given by

$$f(\mu, E) = \left(e^{(E-\mu)/k_B T} + 1 \right)^{-1}, \tag{14}$$

where k_B is the Boltzmann constant and μ the chemical potential of the sample. Since the derivative of the Fermi–Dirac function is a strongly peaked function of E, which vanishes everywhere except for energies close to the chemical potential, μ, the integral will be essentially zero outside an interval of width $k_B T$. The conductance, in general, will be enhanced if the chemical potential is close to a set of transmission peaks (resonances) and reduced when the chemical potential is away from resonant transmission peaks. Thus the conductance as a function of temperature will exhibit several characteristic structures depending on the location of the chemical potential. In our case, since we are just interested in the field dependence of the conductance and the effect of the nonlinear interaction, we will fix our chemical potential to zero in all computations. We should also keep in mind that our energies are counted in units of V, which in general is of the order of few meV. Thus while computing the conductance in Eq. (13) it should be born in mind that temperatures of the order of $T \simeq 10^{-1}$–10^{-2} are reasonably low temperatures while $T \simeq 1$ correspond to high temperatures.

We have calculated the conductance numerically using the transmission coefficient obtained in the previous section. Fig. 3 shows the normalized conductance $G(B)/G(0)$ as a function of $B/k_B T$, for a relatively large, fixed value of U ($U/V = 3$). The dashed lines show the contributions to G stemming from the individual spin channels, while the solid line shows the total conductance. It is clear from this figure that the up spin channel contributes the most to the conductance. The maximum contribution to the conductance occurs at fields $B \leqslant KT$ and is mainly due to the up spin channel. At very large magnetic fields $B \gg KT$ both spin channels will be suppressed and so

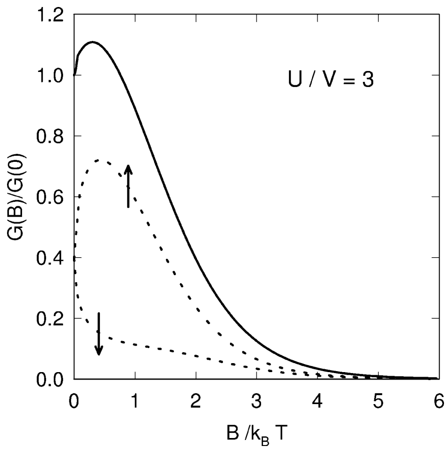

Fig. 3. Normalized conductance versus the applied field, for a relatively high Coulomb correlation energy ($U/V = 3$ and $V_L = V_R = V = 1$). The dashed curves show the contributions from the individual channels while the solid line is the total conductance.

does the conductance as shown in Fig. 3. Thus the magnetic field dependence of the conductance exhibits a clear transition from correlated to uncorrelated transport and the crossover arises when $B \simeq U$. At this stage it is worth mentioning the major difference between the nonlinear impurity problem we have studied in this work and the Anderson impurity problem treated in the literature. The Anderson Hamiltonian treats the system at the quantum level with an on-site Hubbard interaction $Un_\uparrow n_\downarrow$ which in the presence of a magnetic field will lift the degeneracy of the two spin states. Thus in the large U limit and at finite temperature ($B \geqslant kT$) only one spin channel will be available for transport. In this case $G(B)/G(0)$ will have a finite asymptotic value reflecting the blockage of one of the spin channels. In our case the Coulomb interaction is weighted by the probability amplitude $|\Psi_{0\sigma}|^2$ and, due to the continuous nature of this amplitude, the Coulomb effect will be averaged out.

5. Conclusion

We have studied in this Letter a simple alternative model for the transmission properties of a single magnetic impurity embedded in a perfect chain and subject to a static magnetic field, based on an extension of the DNLS equation. The results show that the transmission for an electron with spin parallel to the external field is always greater than the transmission for the antiparallel spin. This result is in accord with the Hubbard model and kinetic equation approaches and reflects the strong Coulomb correlation in the system. Contrary to what is usually observed in one-impurity problems, the transmission across our magnetic impurity does show the existence of resonances, for a range of magnetic fields $0 < B/V < 1/\sqrt{2}$ and correlation energies $0 < U/V < 3/\sqrt{2}$. A completely reflectionless mode has also been observed in the problem of a ferromagnetic Heisenberg chain with a nonlinear anisotropic impurity [14]. The normalized conductance $G(B)/G(0)$ shows a single maximum as a function of the external field intensity, which occurs at relatively low field intensities, then it decreases quickly at large fields.

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