A Self-consistent Hartree Approach to Nonlinear Transport

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PACS number(s): 71.55.-i, 72.10.Fk, 73.40.Gk, 73.20.Jc

Abstract

Using a spin dependent discrete nonlinear Schrodinger equation (DNLSE) we study the transport properties of a single nonlinear impurity connected to two perfect leads. The charge build up at the impurity site is taken into account through the use of a self consistent Hartree mean field approach. The transmission and conductance through the localized impurity is being considered in the presence of both local nonlinear interaction and a magnetic field which lifts the spin degeneracy at the impurity site.

Key words: Charging; Nonlinearity; Magnet-Conductance;

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1 Introduction

In studying the transport properties through mesoscopic devices Spin-Dependent Electron-Electron Interaction (SDEEI), is one of the main sources of nonlinearity that must be considered when solving the Schrödinger Equation [1]. Considering such nonlinearities, the modified version of this equation is known as the Discrete Nonlinear Sch$\ddot{o}$rdinger Equation (DNLSE) which provided greate insight into many physical systems ranging from polaron and soliton related problems to nonlinear electrical and optical problems in quantum nanostructure devices [2]. In the case of SDEEI, nonlinearity studies revealed some interesting properties, like non-vanishing magneto-conductance, which are of great importance in technology. In our present work, the SDEEI is the main source of nonlinearity in the Schrodinger equation describing a single impurity, or under certain special conditions a quantum dot [3], in an infinite tight binding (TB) Hamiltonian system. This system is similar to the one studied in reference [1] but with charge build up effects included by solving the problem self-consistently [4]. This is an essential modification to the previous model since in nano-structures, like semiconductor quantum dots, the dominant contribution to the capacitance charging energy arises from the on-site Coulomb repulsion. This repulsion is a dynamical property of the nano-structure, or impurity, that cannot be considered fixed over time or possible statistical configurations of the system as was assumed previously. Intuitively, it should increase as charge builds up inside the nano-structure device and this should affect the dynamics of the system significantly. From the experimental point of view the physical dimensions of these nano-structures have reached levels such that their capacitance can be as small as 10^{-16} F which can give rise to a Coulomb charging energy $E_c = e^2/2C \simeq 0.1$ meV much larger than the energy spacing between the single particle states of the quantum structure or impurity. Under these conditions, the interplay between Coulomb interaction and energy quantization plays a decisive role in the explanation of the main properties of these nano-structure devices [5].

In this paper, we will extend the results found in a previous work by one of the authors [1] by including charge build up effects through a self-consistent technique first introduced by Cota et al [4] in the context of the general Coulomb electron-electron interaction. Their results showed the charge build up clearly in a quantum dot system along with its other manifestations like the resonance energy shifts and narrowing of the resonance widths. Even though the origin of the electron-electron interaction is different in our model from that of Cota, we still use the same form of the DNLSE. In contrast to Cota's case where a single DNLSE was used to solve the problem, in our case, two coupled DNLSE's will be used self-consistently one for each of the spin states. This shows that correlation effects between the two spin states play an important role and are included from the outset in our mean field model.

Furthermore, Confinement and Contact effects (with leads) were also excluded in our model to concentrate only on the charging effects.

The rest of our paper is organized as follows. In Section 2 we introduce our model and derive the main equations used in this numerical study. In section 3 we provide our main results by evaluating numerically the transmission and conductance of our system along with the magneto-conductance. In the last section we present our conclusions with a summary of the main results.

2 Theoretical Model

The model we consider 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 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. This is a simple model that exhibits electron spin correlations which will have some drastic consequences on the transport properties. The DNLSE describing our system reads [4]

$$i\frac{d}{dt}\Psi_{n,\sigma} + \sum_m V_{n,m}\Psi_{m,\sigma} + (\,\epsilon_{n,\sigma} + U\delta_{n,0}\;\rho_n\,)\Psi_{n,\sigma} = 0. \qquad (1)$$

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. Thus, $\epsilon_{0,\sigma}$ is the local energy at the impurity site. $V_{n,m}$ is the overlap integral which in general, depends only on the distance between the two sites m and n, so that $V_{n,m} = V_{m,n}$. U is a parameter measuring the strength of the local Coulomb interaction. This repulsive interaction arises from the charge accumulation at the impurity site 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 quantum level. The main results of this paper are pivoted around replacing the electronic charge Single State Local Density (SSLD) $\rho_{n-\sigma} =\mid \Psi_{n-\sigma}(E) \mid^2$, which was used in previous studies of this model, by the average local density defined through the density of states $g(E)$ in the infinite TB system. Now E plays the role of Fermi energy for the many body problem and the incident electron at the Fermi level will have to interact via Coulomb interaction with all occupied states below the Fermi level. Contrary to previous approach [1] where we considered a single orbital problem and consequently the incident electron interacts via Coulomb interaction only with opposite spin due to Pauli principle. Thus the new *Average* Local Density (ALD) is given by:

$$\rho_n = \sum_\sigma \int_{-2}^{E} g(E') \mid \Psi_{n\sigma}(E') \mid^2 dE'. \tag{2}$$

Thus in this Hartree approximation the incident electron feels the effective on-site energy $U\rho_n(E)$ which is positive, so that the whole spectrum moves upward in energy. In this approach the nonlinear term is described not by a single orbit of the incident electron like in our previous work [1] but rather by the sum of all orbits below the Fermi energy (strictly speaking the energy of the incident electron because Fermi energy is not defined for a single electron problem). This approach is then by necessity a mean field approach which howerver allows for more than a single orbital and it is very suitable for the implementation of charging effect.

The modified DNLSE includes self-consistency by replacing the previous local density with this *average* one. Let us find the stationary states of (1), 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 n-th and the $(n+1)$-th site, then under these assumptions our previous equation becomes

$$(E - \epsilon_{n,\sigma})\Psi_{n,\sigma} = V_{n,n-1}\Psi_{n-1,\sigma} + V_{n,n+1}\Psi_{n+1,\sigma} + \delta_{n,0}\, U\rho_n\Psi_{n,\sigma}. \tag{3}$$

Since we are not interested in the effect of the leads on the transmission properties of the system we choose the hopping integrals to be unity all over our system.

3 Transmission Coefficient and Conductance

To study the scattering properties of our system we send a plane wave from the left lead towards the nonlinear magnetic impurity located at the origin ($n = 0$) and study its transmission. Thus, we assume that our solution has the following asymptotic form

$$\Psi_{n,\sigma} = \begin{cases} (I_\sigma e^{ikn} + R_\sigma e^{-ikn})\chi_\sigma & for\;\; n \leq -1 \\ T_\sigma e^{ikn}\chi_\sigma & for\;\; n \geq 1 \end{cases}. \tag{4}$$

Where I_σ, R_σ and T_σ are the amplitudes of the incident, reflected and transmitted parts of the wave, respectively. The quantity χ_σ describes the electronic spin state which is assumed to be conserved all along the transmission process since we are ignoring spin flip. Inserting Eq.(4) into Eq.(3) for n=0, ± 1, and after using the lead's dispersion relation $E = 2V\cos(k)$, where the on-site energies are 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

$$\tau_\sigma = \frac{4\sin^2 k}{\left|\left(2\cos k - \epsilon_{0,\sigma} - U\int_0^E \tau_{-\sigma}|I_{-\sigma}|^2 g(E')dE'\right) - 2e^{ik}\right|^2} \tag{5}$$

We note that the incident wave amplitude $|I_{-\sigma}|$ renormalizes the nonlinearity term to an effective Coulomb strength $U_{eff} = U|I_{-\sigma}|^2$. Since we are not interested in renormalization effects due to the incident wave, we set the amplitude of the incident wave to unity independently of the spin, $|I_\sigma|^2 = 1$. This simplifying assumption will not affect the conclusions of our present work. Note that not only we have a nonlinear transmission in this problem, 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 equation (5). It is implicit in this last equation that $\tau_\sigma = \tau_\sigma(E)$ depends on the energy of the incident electron.

We obtained our results using two independent numerical methods. The first method is by solving equation (5) self-consistently. This method is the main method used in producing the results of this paper since it turned out to be faster. We also used the iteration method defined by equation (3) which gave similar results and served as a numerical check. 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. The transmission is found by numerically solving equation (5). Figure 1 shows the transmission as a function of energy for different values of the nonlinearity at zero magnetic field. The persistence of the resonance at the center of the energy band is clear from this figure. This result is expected since the local density defined by (2) vanishes at the center of the energy band and hence leads to the vanishing of the nonlinear interaction. As the nonlinearity increases, the energy band width for transmission decreases significantly but remains symmetric around the center of the band. We also need to point out that due to our choice of parameters where are all overlap integrals are taken to be unity and consequently the impurity is strongly coupled to the leads resulted in a broad transmission curve as shown in Figure 1.

As the magnetic field is introduced, the spin degeneracy is lifted and the symmetry of the transmission is broken as is evident in Figure 2. The fact that the magnetic field lowers the local energy of the up spins and increases the energy of the down spins plays an important role in the transport properties of the spin channels. In Figure 2, spin down and spin up transmissions are shifted towards the negative and positive energy band regions, respectively. However these transmission curves are almost completely symmetric by reflection with respect to the center of the energy band. This gives rise to a vanishingly small zero temperature magneto-conductance (ZTMC). This is a major correction to previous study related to the SSLD case [1] where the ZTMC was found to be finite. Resonances in transmission at certain values of the magnetic field still exist in the ALD case as shown in Figure 4, albeit extra work is required to investigate them. This is so since resonances are not easily tractable as in the SSLD case where they could be found using a closed form formula based on a simpler version of equation (5).

The conductance spin polarization (also called magneto-conductance) is defined by $\Delta G = G_\uparrow - G_\downarrow$ where G_σ is the two-probe conductance (in units of $2e^2/\hbar$) for a single spin channel at finite temperature and is defined by the thermal average of the transmission coefficient [6]

$$G_\sigma(T,\mu) = \int \left(-\frac{\partial f(\mu,E)}{\partial E} \right) \tau_\sigma(E) dE. \tag{6}$$

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

$$f(\mu,E) = \left(e^{(E-\mu)/k_B T} + 1 \right)^{-1}, \tag{7}$$

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.(6) 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 from equation 5. At very large temperatures $T \gg B$ (

recall that we set Boltzmann constant to unity) both spin channels will be suppressed and so does the conductance as shown in Figure 3. At low temperatures the up spin conductance dominates the transport while the down spin conductance is negligible as shown in the above figure. Thus at low temperatures we observe a substantial magneto-conductance as shown in Figure 4. Such an effect can play an important role in spin sensor applications in nano-structure devices. As the nonlinearity increases, both spin conductance channels approach zero. Its maximum increases with nonlinearity and shifts towards higher values of the magnetic field, this also reflects the fact that this the origin of this huge magneto-conductance is purely a nonlinear effect as shown in the inset of figure 4.

4 Conclusion

We have studied the effect of spin dependent charging effect on the transport properties of a single nonlinear impurity model using a self consistent approach that ensures the good implementation of the nonlinear Coulomb interaction term. The Discrete Non-Linear Schrodinger Equation(DNLSE) was used to investigate the effect of charge build up on the transmission and conductance of a single magnetic impurity system embedded in an infinite tight binding hamiltonian. Charge build up has been shown to change the transmission properties drastically due to the Zeeman effect which lifts the degeneracy of impurity energy levels giving rise to major differences in the zero temperature limit of the conductances . This in turn gave rise to huge differences in the linear magneto-conductance of the system. In the ALD case, the zero temperature magneto-conductance was shown to be vanishingly small for large values of the nonlinearity in contrast to the SSLD case where it is finite and substantial. The ALD case can be seen as an important correction to the SSLD case and the behavior of the conductances it predicts is more trustworthy.

5 Acknowledgments

We would like to thank the physics department at KFUPM for its continuous support during the progress of this work.

References

[1] M. I. Molina and H. Bahlouli, Phys. Lett. A 294 , 87-94 (2002)

[2] 'Disorder with Nonlinearity', eds. F. Abdullaev, A.R. Bishop and S. Pnevmatikov, Springer-Verlag, Berlin, (1992) and D. Hennig and G. P. Tsinoris, Phys. Rep. Vol. 307, 333 (1999).

[3] Y. Meir, N. S. Wingreen and P. A. Lee, Phys. Rev. Lett. 66, 3408 (1991); A. Groshlev, T. Ivanov and V. Valtchinov, Phys. Rev. Lett. 66, 1082 (1991).

[4] E. Cota and S. E. Ulloa, Phys. Rev. B 51 , 10875 (1995)

[5] D. V. Averin and K. K. Likharev, in Mesoscopic Phenomena in Solids, edited by B. L. Altshuler, P.A. Lee and R. A. Webb, Elsevier, Amsterdam (1991).

[6] M. Ya Azbel, A. Harstein and D. P. DiVincenzo, Phys. Rev. Lett. 52, 1641 (1984).

Fig. 1. Transmission versus energy at zero magnetic field for different values of the nonlinearity parameter U.

Fig. 2. Transmission versus energy for a nonlinearity parameter U = 3 and magnetic field B = 0.5.

Fig. 3. Spin down, spin up and total conductance versus magnetic field for temperature T=0.1 and nonlinearity parameter U = 3.

Fig. 4. The magneto-conductance versus magnetic field for temperature T=0.1 and different values of the nonlinearity parameter U.