Transport Through a Small Interacting System

H. Bahlouli*

Physics Department, KFUPM, Dhahran 31261, Saudi Arabia.

Abstract

We study the effect of nonlinear interaction, and finite coupling, V_0, to the leads on the transmission properties of a finite 1D chain of N atoms. The two-probe dc conductance, G, through a finite interacting chain connected to reservoirs is studied both in the $T = 0$ and $T \neq 0$ cases. At T = 0 we observe that, for E = 0, perfect transmission occurs for odd values of N while for even N, the transmission reaches its minimum value. This results in an even-odd oscillatory behavior which becomes suppressed at higher temperatures. The two-probe conductance is also seen to be drastically reduced when the strength of the nonlinear interaction, U, is of the order of the inter-site coupling.

PACS numbers: 72.15.N, 71.10.F, 73.61

*Email bahlouli@kfupm.edu.sa

1 Introduction

Electronic transport in low dimensional systems is a subject of recent interest due to its importance in the physics of nanostructure devices [1] which have a huge potential application in the future electronic and opto-electronic devices. Progress has been especially rapid in recent years due to the development of advanced crystal growth and lithography techniques that facilitated sophisticated experiments at the nanoscale level [2]. Apart from their potential use as novel devices, such systems are also interesting from a fundamental physics point of view. Because of their finite size, the electronic properties of these nanostructures will most likely dependent on the size of the system, on the interaction between electrons and on the strength of the confining potential.

When electrons are confined to a small region of a semiconductor they form a quantum dot. Quantum dots are small islands of electrons that are governed by the interplay of quantum mechanical and electrostatic effects. By trapping electrons in a zero dimensional quantum dot a complete quantization of the electron's free motion is realized and the charge on the dot is also quantized. It is now possible to control their shape, dimensions, the structure of the energy levels, and the number of confined electrons. Often, quantum dots are referred to as " artificial atoms " because electronic states within closed dots are quantized, permitting spectroscopic measurements [2]. Conductance studies have demonstrated that transport through a small confined electron gas or quantum dot is strongly regulated by Coulomb interaction [3]. It is possible to study the transmission of electrons through a quantum dot by coupling the states in the dot to external leads via tunnel barrier. Furthermore the charge on the dot is quantized and can be controlled by a nearby metallic gate. The discrete charging energy gives rise to the phenomenon of Coulomb blockade, which manifests itself in the form of periodic peaks in the transmission (or two probe conductance) as a function of gate voltage. This phenomenon has been under intensive study in recent years.

It is known that the electron-electron interaction is important in any serious study of the transport properties of small systems such as quantum dots and finite quantum wires [4]. The Coulomb interaction, generally speaking, gives rise to a nonlinear term in the Schrodinger equation. In this case the Coulomb interaction is modeled by a cubic non local term in the equation of motion of the corresponding fermionic field operators. To pro-

ceed further a Hartree-Fock approximation for the nonlinear term is used [5]. One can also use a perturbative approach in the Coulomb interaction [6]. In my present study I take the alternative approach of studying the effect of the electron-electron interaction as being modeled by a nonlinear local term in the Schrodinger equation. One can look at such an approximation as being a Hatree like approximation of the original many body problem. Besides its relevance to our electronic systems, the nonlinear interaction was also a subject of intensive research both from the theoretical and experimental point of view [7] because of its importance in optical and electronic devices. In particular it has been shown that nonlinearity gives rise to multistability , noise and might originate a chaotic behavior in certain systems. Recently, transport properties of nonlinear chain of atoms and double barrier structures under applied electric fields have been examined [8]. In their work Cota et al. [8] showed that the resonances shift in the presence of nonlinearity and that their width decreases as the nonlinearity becomes stronger.

In this paper we report on the numerical calculation of the two-probe conductance and the transmission coefficient of a finite interacting 1d system connected to two perfect leads. Since in our present study we are not concerned with the charging effect, which is of primary importance for quantum dots, we will not take into consideration the confining potential of the chain. In section 2 we introduce our model and explain the principle of our numerical approach. In section 3 we evaluate the transmission coefficient both in the presence and absence of nonlinear interaction. In section 4 we present the numerical results of the finite temperature conductance and study the effect of the on site Coulomb interaction on the conducting properties of the finite chain. Finally in section 5 we present our conclusions with a summary of our basic results.

2 Theoretical Model

In this letter we would like to investigate the effect of the on site nonlinear interaction on the transmissive properties of a tight binding system described by Anderson hamiltonian. We use the standard Anderson model to describe this system . The model consists of three regions (see Fig.1) ; a finite chain at sites $1 \leq i \leq N+1$, and two semi-infinite leads on the left $-\infty < i \leq 0$, and the right $N+2 \leq i < +\infty$. The nonlinear Schrodinger equation we will be studying in this work is derivable from the following

discrete Hamiltonian

$$H = \sum_n \left[\epsilon_n \Psi_n^* \Psi_n + \sum_{m \neq n} V_{n,m} \Psi_n^* \Psi_m + \frac{1}{2} U \mid \Psi_n \mid^4 \right] \tag{1}$$

where $\Psi_n(t)$ is the complex amplitude and ϵ_n the energy at site n (n = 1,2,$\cdots$, N+1, N being the size of the chain). U is the strength of the on-site interaction within the chain and $V_{n,m}$ is the overlap integral which depends, in general, only on the distance between the two sites m and n, so that $V_{n,m} = V_{m,n}$. Note that Ψ_n and $i\Psi_n^*$ form canonically conjugate variables and $\frac{d}{dt}\Psi_n = -\frac{\partial H}{\partial (i\Psi_n^*)}$ is the corresponding equation of motion. From the above Hamiltonian we then obtain

$$i\frac{d}{dt}\Psi_n = \sum_{m \neq n} V_{n,m}\Psi_m + (\epsilon_n + U \mid \Psi_n \mid^2)\Psi_n \tag{2}$$

Our theoretical model (2), which is basically an effective one electron problem, does not yield an exact solution of the actual many electron system representing nanostructure devices. The Coulomb interaction between confined electrons is a long range interaction. So our model (2) does not correspond to the well known Hubbard model, which is often used as a model hamiltonian describing nanostructure devices. Nevertheless, the nonlinear discrete Schrodinger equation (2) contains some essential features of the interacting system, that is, the repulsive and nonlinear nature of the interaction.

Let us study the stationary states of the above nonlinear Schrodinger equation i.e. we look for solutions of the type $\Psi_n(t) = e^{-iEt}\Psi_n(E)$ where E is the associated eigenvalue. We restrict ourselves to the tight-binding approximation, where only nearest neighbor hopping is allowed for. Let $V_{n,n+1}$ be the hopping integral between the n-th and the (n+1)-th site, then under these approximations our previous equation becomes

$$(E - \epsilon_n)\Psi_n = V_{n,n-1}\Psi_{n-1} + V_{n,n+1}\Psi_{n+1} + U|\Psi_n|^2\Psi_n \tag{3}$$

where the hopping integrals are defined by

$$V_{n,n+1} = \begin{cases} V_L & for \;\; n < 0 \;\; or \;\; n \geq N+2 \\ V_0 & for \;\; n = 0 \;\; and \;\; n = N+1 \\ V_S & for \;\; 1 \leq n \leq N \end{cases} \tag{4}$$

The hopping matrix element within the leads is denoted by V_L, the link between the leads and our system is described by the hopping matrix element V_0 while hopping within the system is described by V_S. Before going

any further let me mention that the above discrete nonlinear Schrodinger equation (DNSE) can be derived, in principle, from the more general nonlinear Schrodinger equation $i\partial_t\Psi + \partial_x^2\Psi + f(x, \mid \Psi \mid^2)\Psi = 0$. The function $f(x, \mid \Psi \mid^2)$ characterizes the effective self-interaction of the quasiparticles in the system. It is important to point out that our nonlinear Schrodinger equation model defined by equation (3) does not correspond exactly to the classical Hartree approximation of the Hubbard model. In the Hartree approximation of the Hubbard model the nonlinear term is described not by a single orbit as described in equation (3) but rather by the sum of all orbits below the Fermi level.

From the computational point of view equation (3) is very useful, it relates the values of the wave function at three successive discrete locations along the x-axis, it is often referred to as Poincare map in the literature [10, 9]. For one dimensional systems the discretization of the Schrodinger equation can be performed exactly [9]. The solution of equation (3) is done iteratively by taking our initial conditions $\Psi_0 = 1$ and $\Psi_{-1} = \exp(ik)$, the lattice spacing is set to unity all along this article. We consider here an electron having a wave vector k incident at site N+2 from the right (by taking the length of chain L = N, i.e. N+1 sites) the transmission coefficient can then be expressed as [10, 11]

$$T = \frac{4\sin^2 k}{\left|\Psi_{N+2} - \Psi_{N+3}\exp(-ik)\right|^2} \tag{5}$$

Thus the transmission coefficient depends only on the values of the wave function at the end sites, Ψ_{N+2} , Ψ_{N+3} which are evaluated from the iterative equation (3). In the region outside the chain, the leads are described by a non-interacting tight-binding hamiltonian for which the dispersion relation reads

$$E = 2V_L cosk \tag{6}$$

which relates the incident electronic energy, E, to the propagation wave number k. For convenience, we measure all energies in units of V_L, i.e. we set $V_L = 1$ in our numerical computations.

3 Transmission Coefficient

We consider first the problem of transmission of an electron incident on a quantum wire where the nonlinear interaction is neglected. In this case

our previous equation reduces to

$$(E-\epsilon_n)\Psi_n = V_{n,n-1}\Psi_{n-1} + V_{n,n+1}\Psi_{n+1} \tag{7}$$

In the absence of nonlinear interaction the system is symmetric with respect to left-right exchange so that we can assume unit transmission and iterate to get the incident amplitude. We assume an incident wave having an energy E, when it passes through our sample part of it will be transmitted and part of it will be reflected so that one can write for the wave amplitude

$$\Psi_n = \begin{cases} e^{ikn} + Re^{-ikn} & for \;\; n \leq 1 \\ Te^{ikn} & for \;\; n \geq N+1 \end{cases} \tag{8}$$

the wave vector k is defined through the semi-infinite leads dispersion $E = 2V_L \cos k$, within the system the propagation wave vector is also assumed to obey a similar dispersion $E = 2V_S \cos k_1$. The on site energy ϵ_n is taken to be zero for simplicity. After a small exercise using the transfer matrix method we find the following result [12].

$$\begin{aligned} |T|^2 &= \frac{A}{4\left[B\sin(k_1 L) + C\sin(k_1(L-1))\right]^2 + A} \\ A &= (4 - \frac{E^2}{V_L^2})(4 - \frac{E^2}{V_S^2}) \\ B &= \frac{V_L}{V_S}\left(\frac{E^2}{V_0^2} - \frac{E^2}{V_L^2} + \frac{V_0^2}{V_L^2} - \frac{V_S^2}{V_0^2}\right) \\ C &= \left(1 - \frac{V_L^2}{V_0^2}\right)\frac{E}{V_L} \end{aligned} \tag{9}$$

Clearly when $V_S = V_L = V_0$ the transmission is unity as expected irrespective of the sample length. We would like to study the behavior of this transmission as a function of V_0 . We notice first of all that this two probe conductance ($G = |T|^2$ in units of $2e^2/\hbar$, where the factor of 2 takes the spin into account) has an oscillatory behavior as a function of L. This oscillatory behavior originates from the sinusoidal length dependence of the denominator in the transmission coefficient (9). We have plotted in Fig.2 the transmission coefficient as a function of energy for even and odd N. This figure shows clearly that the Fermi level ($\mu = 0$) is located at the maximum of the transmission for odd N and at the valley for even N. Thus as the length

grows from even to odd values, the conductance jumps from a point on the even pattern to the next on the odd pattern or vise versa. This oscillatory behavior of the two probe conductance is a characteristic of ballistic systems. Also we should expect that the amplitude of this even-odd oscillations to depend strongly on the energy of the incident electron and on the magnitude of the interaction with the leads, V_0. This feature can be easily seen from (9) if we set E = 0 (thus $k_1 = \pi/2$) then the transmission becomes unity for odd lengths and has a finite value, which depends on V_0, for even lengths.

Now let us turn to the interacting system described by (3). In Fig.3 we show the effect of the nonlinear interaction on the transmission coefficient for N = 4, U = 0.02, $V_S = 1$ and $V_0 = 0.2$. It is clear that the resonance are shifted to higher energies while their width is being reduced compared to the non-interacting case (continuous line). Since the nonlinear interaction term in equation (3) is positive, the incident electron feels the effective on site energy $U \mid \Psi_n \mid^2$ which is positive, so that the spectrum moves upward in energy.

4 Coulomb Interaction and Temperature Effects on the Conductance

In order to obtain a realistic picture of our model, it is convinient 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]

$$G(T,\mu) = \int \left(-\frac{\partial f(\mu, E)}{\partial E} \right) |T(E)|^2 \tag{10}$$

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

$$f(\mu, E) = \left(e^{(E-\mu)/kT} + 1 \right)^{-1} \tag{11}$$

k 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 kT. Thus one should expect strong variations of the conductance with variations in the chemical potential. 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 thermal effect on the even-odd oscillatory behavior and the effect of the nonlinear interaction on the conductance 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_L, which in general is of the order of few meV. Thus while computing the conductance in (10) 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 sections. In Fig.4 we show the behavior of the conductance for U = 0., $V_S = 1$, $V_0 = 0.4$, $\mu = 0$ and T = 0.1. It is clear from this figure that the even-odd oscillations are damped due to the energy integration over kT range at finite temperature. Thus the oscillatory behavior at finite temperature survives only at small length scales as seen in figure 4. In Fig.5 we study the behavior of the conductance as a function of the sample length for V_S =2, V_0 =0.5, μ =0, T =0.02 and U = 0.1. As expected the repulsive nonlinear interaction tends to localize the electronic states and consequently will reduce the conductance in general. From this figure we note two important signatures, one is the decay of the oscillatory behavior of the conductance which is presumably due to thermal fluctuations similarly to what happened in Fig.4, we call this feature the thermal decay envelop. Second, within this thermal decay envelop we observe an oscillatory behavior which is certainly due to the nonlinear interaction. The explanation of this observation is not trivial. We have a resonant behavior of the conductance which is damped by thermal effects. We know that the number of resonances is length dependent, whenever the length increases the number of resonances also increases. At these resonances the transmission is maximum but in order for this resonance to give a substantial contribution to the conductance we need the resonant energy to be very close (within kT) to the chemical potential set to be zero in our computation. Now from our recursive relation (3) we realize that under the action of a nonlinear interaction we can define an effective energy $\tilde{E} = E - U \mid \Psi_n \mid^2$ for our traveling electron. At the resonant energies of the chain the effect of the nonlinearity is to shift approximately these resonances to the right and reduce their width

as can be seen from Fig.3. Thus at certain lengths when one resonant level coincides with the chemical potential ($\mu = 0$) the conductance will resonates while increasing the length a little more puts this resonance off the chemical potential and consequently reduces its contribution to the conductance. Increasing the length a little more will bring another to coincide with the chemical potential and makes the conductance resonate, but with less magnitude because the resonance width has been reduced, and so on. In Fig.6 we present the behavior of the conductance as a function of the strength of the nonlinear interaction U normalized to its non-interacting value G(U = 0). We see from this figure that the magnitude of the conductance decreases sharply when the Coulomb interaction becomes comparable to the inter-site hopping energy, set to unity in our computations ($V_0 = V_S = 1$).

5 Conclusion

We have studied in this article the effect of a nonlinear interaction on the transmissive properties of a finite one dimensional system. An atomic chain of N interacting atoms connected to two semi-infinite non-interacting leads. At T = 0 and in the absence of nonlinear interaction we have found that the system displays an even-odd oscillatory behavior in the linear conductance. These oscillations are strongly energy dependent and occur whenever the energy of the incident electron coincides with one of the resonances of the finite chain. For instance if the energy of the incident electron is set to E = 0, then for odd N, the isolated chain has an eigenstate at E = 0 (Fermi level), which will give rise to a resonant state when coupled to the leads and hence contributes to perfect transmission. On the other hand, for even N, there is no discrete eigenstate at E = 0 for the isolated chain and consequently no perfect transmission will arise for the coupled chain. A similar behavior is also observed at other resonant energies of the finite chain. At finite temperatures, this even-odd oscillation is eventually damped due to thermal fluctuations, the even-odd oscillations survive only for small samples in this case. The finite temperature two probe conductance is also observed to be reduced drastically when the Coulomb interaction is of the order of the inter-site hopping energy. Thus the even-odd oscillatory behavior is sensitive to many parameters in the model. In particular it is very sensitive to the strength of the coupling to the leads, to the temperature and the strength of the nonlinear interaction. Our results are in qualitative

agreement with the recent computations of Oguri [6] using a perturbative Green function approach at T = 0 and the finite temperature calculations for non-interacting quantum wire considered by Yamaguchi et al. [14] using a T-matrix approach. This agreement by itself constitutes a strong support to the fact the discrete nonlinear Schrodinger equation captures some of the most important features of the interacting system.

Acknowledgements

I would like to acknowledge the support of King Fahd University of Petroleum and Minerals during the progress of this work.

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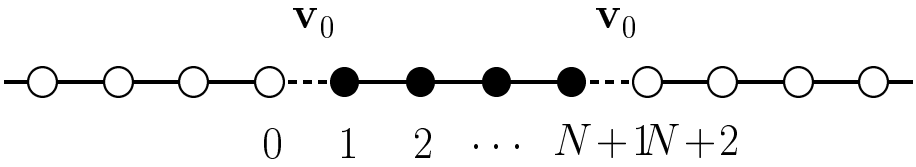

Fig. 1

Figure Captions

Fig.1

Schematic picture of the model: (•) interacting region, (∘) noninteracting leads.

Fig.2
The transmission coefficient versus energy for U = 0., $V_S = 1$, $V_0 = 0.4$, N = 10 (continuous) and N = 11 (dots).

Fig.3
The transmission coefficient versus energy for V_S= 1, $V_0 = 0.2$, N = 4, U = 0.02 (dots) and U = 0 (continuous).

Fig.4
The normalized conductance versus length for U = 0., $V_S = 1$, $V_0 = 0.4$, μ = 0 and T = 0.1 .

Fig.5
The normalized conductance versus length for $V_S = 2$, $V_0 = 0.5$, $\mu = 0$, T = 0.02 and U = 0.1.

Fig.6
The normalized conductance versus the strength of the Coulomb interaction U for $V_S = V_0 = 1$, E = $\mu = 0$, N = 2 and T = 0.4 .