Electron correlation effects in the presence of non-symmetry dictated nodes

P SINGHA DEO

S.N. Bose National Centre for Basic Sciences, J.D. Block, Sector III, Salt Lake City, Kolkata 700 098, India

Abstract. We numerically study the effect of non-symmetry dictated nodes (NSDN) on electron correlation effects for spinless electrons. We find that repulsive interaction between electrons can enhance the overlap between nearest neighbors in the tight binding Hamiltonian, in the presence of NSDN. Normally, in the absence of NSDN, attractive interaction between electrons give such an effect and repulsive interaction gives the opposite effect.

At low temperatures, inelastic collisions are greatly suppressed. As a result the phase coherence length of an electron can become a few microns. Mesoscopic systems are defined as systems in which the phase coherence length exceeds the sample size. In such a system elastic scattering is the dominant feature and such mesoscopic samples can be understood as phase coherent elastic scatterers. Recently a new kind of scattering phase shift was discussed in Q1D, in connection with the violation of the parity effect [1]. To explain this phase shift and the violation of parity effect, we first explain what are symmetry dictated nodes (SDN) and non-symmetry dictated nodes (NSDN) that can arise in a Q1D system.

For example let us consider a rectangular quantum billiard or dot connected to leads by quantum mechanical tunneling as shown in figure 1. The system has reflection symmetry across the x-axis as well as the y-axis. Also the x-y components separate and spanning nodes (nodes that span across the direction of propagation and shown by dashed line in figure 1) as well as non-spanning nodes (shown by dotted line in figure 1) develop in the geometry, dictated by the reflection symmetries. There are various symmetries that give rise to nodes in the wave function and we call them SDN (for example the antisymmetric property of the many-body wave function result in nodes). But if quantum coherence extends to some distance inside the leads then one can model the phase coherent quantum dot as shown in figure 2. Note that in this case also reflection symmetry holds in the x-direction as well as in the y-direction, but x-y components do not separate. So by tuning the boundary condition in the y-direction by a gate voltage one can develop nodes that try to develop across y-direction but also act across x-direction and change the phase of the wave function in x-direction by π. We call them NSDN because they do not originate due to the symmetry of the Hamiltonian but instead originates due to the boundary conditions.

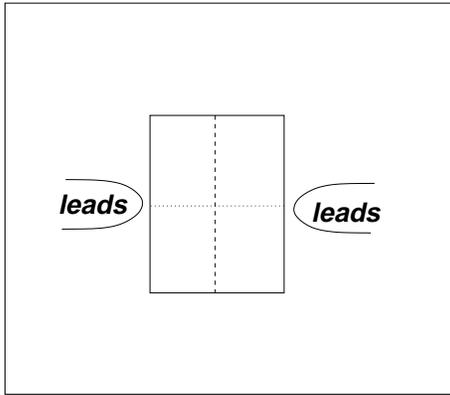**Figure 1.** A rectangular quantum billiard or quantum dot, weakly coupled to leads. The dotted line is along the *x*-axis and the dashed line is along the *y*-axis.
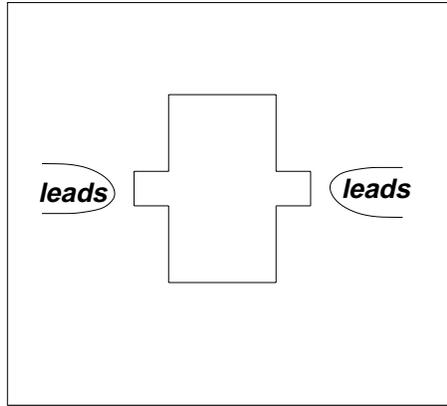
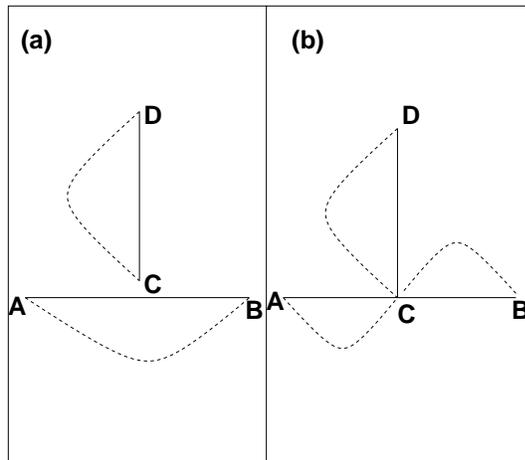**Figure 2.** A more realistic model for the quantum dot of figure 1.

Figure 3. Two one dimensional quantum wires of equal lengths, AB and CD, shown by solid lines, placed along x and y directions, respectively. The origin ($x = 0$, $y = 0$) is at the mid point of AB. (a) CD is not connected to AB. (b) CD is connected to the mid point of AB.

There are many configurations of such NSDN, the simplest one was discussed for the stub geometry (shown in figure 3) in ref. [1], and further elaborated here. Consider for example two finite one-dimensional quantum wires of equal length, AB and CD placed perpendicular to each other as shown in figure 3 by the solid lines. When CD is completely detached from AB as shown in figure 3a, the quantum mechanical wave function in AB and CD in the ground state is shown by the dotted lines. They are basically the ground state wave function in an infinite potential well in one-dimension (1D). As is known to us,

the ground state wave functions are by symmetry, even parity states without any nodes, except at the boundary. But when CD is attached to AB to give a T-shaped stub structure as shown in figure 3b, then CD forms a node at C, which is also the midpoint of AB. The wave function in this case is again shown by dotted lines and the wave function between A and B is no longer an even parity state but an odd parity state. The node at C between A and B does not originate from the symmetry of the Hamiltonian and is not a symmetry dictated node (SDN). It is rather forced by the boundary condition in the y-direction and is a NSDN. An infinitesimal change in the length of CD makes this node disappear and then we have no node between A and B. The node at C induces a phase change by π and when we join A and B together to form a ring-stub system, we also get persistent currents without parity effect, as parity of the persistent currents is sensitive to the number of nodes in the wave function [2].

When semi-infinite leads are attached to A and B in figure 3b then the transmission amplitude of the stub structure has zero-pole pair and one gets Fano resonances [3]. Fano resonances [4] are a very general feature of Q1D [5,6] systems in the presence of defects and the Fano resonances are characterized by a zero-pole pair of the transmission amplitude in the complex energy plane. At the energy corresponding to the pole a charge gets trapped by the scatterer and there is also an energy when there is a zero transmission across the scatterer. At the energy corresponding to the zero transmission, scattering phase shift discontinuously changes by π due to the NSDN [1]. It seems at present that this phase due to NSDN is necessary to understand the experimental results of refs [7–9]. Initial analysis of the experiments in terms of the captured charge and Friedel sum rule [10] revealed the shortcomings of applying Friedel sum rule to the quantum dot. The phase change due to NSDN can explain the experimental data, that was first proposed in ref. [11] and later discussed in refs [6,12–16]. Friedel sum rule in the presence of this NSDN has also been generalized in refs [14,15,17].

In this work we intend to show that this NSDN greatly affects electron correlation effects. We will concentrate on the situation when we have NSDN in the ring-stub geometry, that is when points A and B in figure 3b are joined together to form a ring ACB coupled to a stub CD. In order to diagonalize the electronic Hamiltonian (unlike ref. [18] where we are not interested in the positive charges and polarization) we will consider a lattice Hamiltonian as given below where the ring is made up of three sites (located at A, B and C) and the stub is made up of two sites (located at E and D) (see the inset to figure 4). Such a choice allows a NSDN exactly at the Fermi surface as we shall soon see. The isolated site energies are 0 and ignoring electron spin the Hamiltonian is

$$H = -t\Sigma_{\langle ij\rangle}c_i^+c_j + u\Sigma_{\langle ij\rangle}n_in_j, \tag{1}$$

where c_i is the electron destruction operator at site i, $n_i = c_i^+c_i$ is the operator that gives the occupation probability of site i and $\langle ij\rangle$ means only nearest neighbors are considered in the sum. The two competing energy scales of an interacting electron system are parametrized by t and u. The possible way in which these parameters t and u modify electron correlation effects is known. For positive values, u plays the role of the Coulomb interaction strength between two electrons, that tend to make the electrons avoid each other and localize them as far from each other as possible while t plays the role of the quantum mechanical kinetic energy of the electrons that tends to make the electrons overlap with each other and delocalize. We choose the unit of energy such that $t = 1$, throughout our calculations.
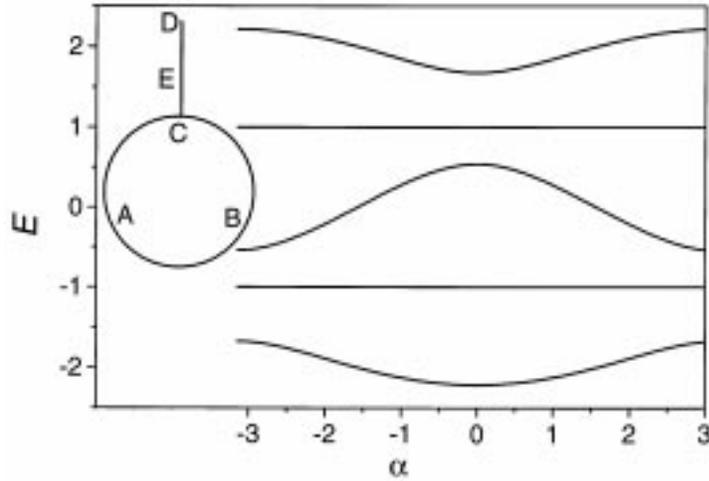
Figure 4. The inset shows a ring-stub geometry. When the ring is made up of three sites and the stub is made up of two sites, then there will be five single particle states in all. The energies (E) of these five states as a function of a dimensionless flux α, through the centre of the ring is shown by the five solid curves.

In figure 4 we plot the single particle energies of the system when $u/t = 0$, as a function of the flux that penetrates through the centre of the ring ABC. It is known that the single particle states will disperse with the flux with a periodicity of $\alpha = 2\pi\phi/\phi_0 = 2\pi$ [19]. Here ϕ is the flux through the ring and $\phi_0 = hc/e$, is the flux quantum. Hence we plot the single particle eigenenergies, which will be five in number (shown by five solid curves) as there are five sites in all, from $\alpha = -\pi$ to $\alpha = \pi$ (i.e. in the first Brillouin zone). The ground state is diamagnetic as expected, i.e. increases in energy with the flux. A striking feature of the spectrum is that two of the states (the first excited state and third excited state) are independent of the flux. This is a purely quantum effect and analysed in ref. [20]. Wave functions in these states have NSDN, similar to what is shown in figure 3b, except that now A and B are joined. Since the node at C is a NSDN, the wave function does not extend across it and so does not enclose the flux and also does not depend on the flux. This does not happen for states with SDN. Hence if we put two electrons or four electrons in the system the NSDN will lie exactly at the Fermi energy. While in a finite system with discrete levels and large separation between single particle levels, one can tune the Fermi energy to coincide with the NSDN only for some special parameter values, it will not be so in a large system or in a system connected to leads.

If we put three electrons in the system then the Fermi surface will be far away from the NSDN and when we switch on u we will expect a competition between t and u. Although the outcome of this competition in the absence of NSDN is well-known, we will demonstrate it here in order to accentuate how the NSDN can change this outcome. For very large positive u one electron stays in the stub and two electrons stay in the ring, there being very little overlap between the stub and the ring. This agree with ref. [18], although the cases that can be studied within the model there corresponds to the two electron case and not the three electron case as considered here. For example, in figure 5 we plot $\langle n_i \rangle$ at sites D

and E versus α for different values of $u > 0$. The dotted curve gives $\langle n_D \rangle$, i.e., expectation value of the operator n_i at the site D when $u/t = 0$. The short-dashed curve gives $\langle n_E \rangle$, i.e., expectation value of the operator n_i at the site E when $u/t = 0$. The solid curve gives $\langle n_D \rangle$, when $u/t = 1$. The dashed curve gives $\langle n_E \rangle$, when $u/t = 1$. The solid curve is greater than the dotted curve at all flux values, i.e., $\langle n_D \rangle$ is enhanced by u, while the dashed curve is less than the short-dashed curve for all flux values, i.e. $\langle n_E \rangle$ is reduced by u. Also note that the enhancement in $\langle n_D \rangle$ is roughly the same as the reduction in $\langle n_E \rangle$ i.e. enhancement in $\langle n_D \rangle$ is at the cost of $\langle n_E \rangle$ and transfer of charge between the stub and the ring is negligible. This means repulsive interaction kills the overlap of the wave function between the sites D and E. For the known competition between t and u, the single electron in the stub is localized and resides almost entirely in the site D.

Opposite effect will be seen for attractive interaction or for negative u. For large attractive interaction all the three electrons will try to cluster together and since the stub is made up of two sites only and cannot accomodate three electrons, for large negative u all the three electrons will stay in the ring. Hence for large and negative u, charge transfer between the ring and the stub becomes dominant and hides the effect that we want to study. But for small negative u i.e. $|u|/t < 1$, interaction will try to enhance the occupation probability at nearest neighbors. For example, in figure 6 we plot $\langle n_i \rangle$ at sites D and E versus α for different values of $u < 0$. The dotted curve gives $\langle n_D \rangle$, when $u/t = 0$. The short-dashed curve gives $\langle n_E \rangle$, when $u/t = 0$. The solid curve gives $\langle n_D \rangle$, when $u/t = -0.5$. The dashed curve gives $\langle n_E \rangle$, when $u/t = -0.5$. The flux values of the solid curve is less than the dotted curve while the values of the dashed curve is greater than the short-dashed curve. So for small values of $u < 0$ one can clearly see that u tends to make $\langle n_E \rangle$ to be roughly equal to $\langle n_D \rangle$, with small deviations due to charge transfer between the ring and the stub, i.e. $\langle n_D \rangle + \langle n_E \rangle$ is not conserved.
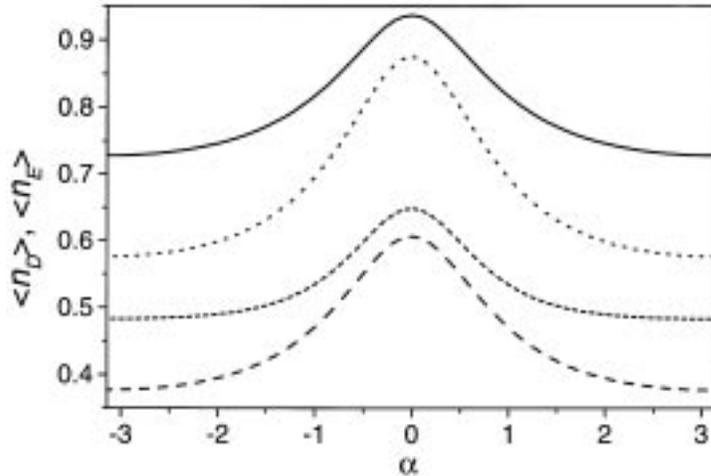

Figure 5. This figure shows the expectation values of the operator for occupation probability at the sites E and D as a function of α. Here $u/t \geq 0$ and there are three electrons in the system.
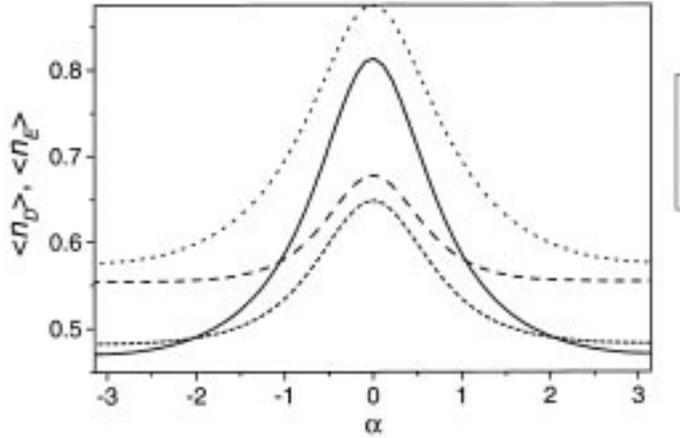
Figure 6. This figure shows the expectation values of the operator for occupation prob-
ability at the sites E and D as a function of α. Here $u/t \leq 0$ and there are three electrons
in the system.

Next we consider the two electron system, i.e. the situation when the NSDN lies at the
Fermi surface. In figure 7 we plot $\langle n_{\text{stub}} \rangle = \langle n_D \rangle + \langle n_E \rangle$ when $u/t = 0$ (solid curve), $u/t = 1$
(dotted curve) and $u/t = 100$ (dashed curve). Note that in the $u/t = 0$ case for $|\alpha| < |\alpha^*|$,
$\langle n_{\text{stub}} \rangle$ is roughly constant in α and then it drops, signifying charge transfer between the
stub and the ring. This is the case studied in ref. [18], however, unlike that in ref. [18],
our calculations are exact and we consider the overlap between all possible states. When
the stub and the ring are decoupled from each other, then the states in the ring will depend
on α but the states of the stub will not. So as a ring state change in energy with α it can
cross a stub state. In case of the parameters used in figure 7, for $|\alpha| < |\alpha^*|$, the isolated
stub ground-state is lower in energy than the isolated ring first-excited-state while it is the
opposite for $|\alpha| > |\alpha^*|$. If the ring and the stub were decoupled, for $|\alpha| < |\alpha^*|$, the total
energy is minimized when we put one electron in the ground state of the isolated stub and
one electron in the ground state of the isolated ring. But for $|\alpha| > |\alpha^*|$, total energy is
minimized if we put both the electrons in the isolated ring, one in the ground state and
the other in the first excited state, the isolated stub being empty. This is why the drop
in $\langle n_{\text{stub}} \rangle$ occurs in the coupled ring-stub system at $|\alpha|=|\alpha^*|$, where of course the kinetic
energy parametrized by t tends to make the isolated ring and isolated stub states overlap,
the overlap being the maximum when the isolated ring state and the isolated stub state
become degenerate at $|\alpha^*|$. Also the NSDN results as a consequence of this degeneracy
between the isolated ring state and the isolated stub state and affects the energetics of the
system specially around $|\alpha^*|$. Now if we switch over to u, then as discussed before, it will
try to destroy the overlap between the ring and the stub states. We can see from figure 7
that when we increase u then $|\alpha^*|$ is pushed more towards the zone boundary and for very
large u once again one electron is localized in the stub and one electron in the ring as if
the stub and the ring are decoupled. One would expect that u will also destroy the overlap
between the sites E and D and the electron in the stub will reside mostly in one of the two
sites as $u \to \infty$. We will show below that actually the opposite happens due to the presence
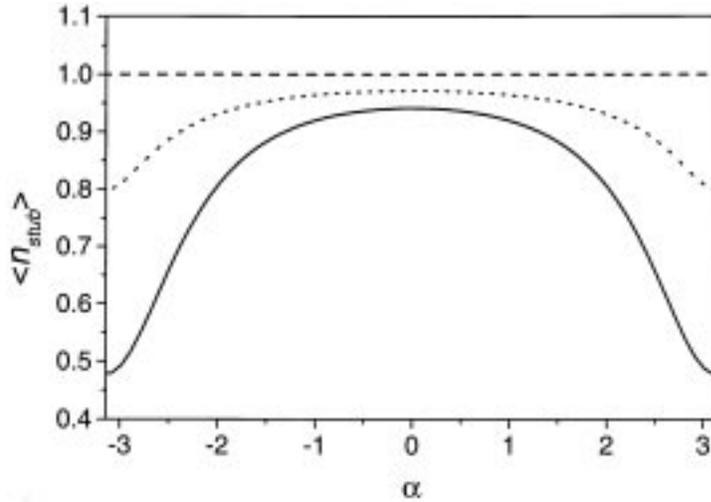of the NSDN.

Figure 7. This figure shows the sum of the expectation values of the operator for occupation probability at the sites E and D as a function of α. Here $u/t \geq 0$ and there are two electrons in the system.

Figure 8. This figure shows the expectation values of the operator for occupation probability at the sites E and D as a function of α. Here $u/t \geq 0$ and there are two electrons in the system.
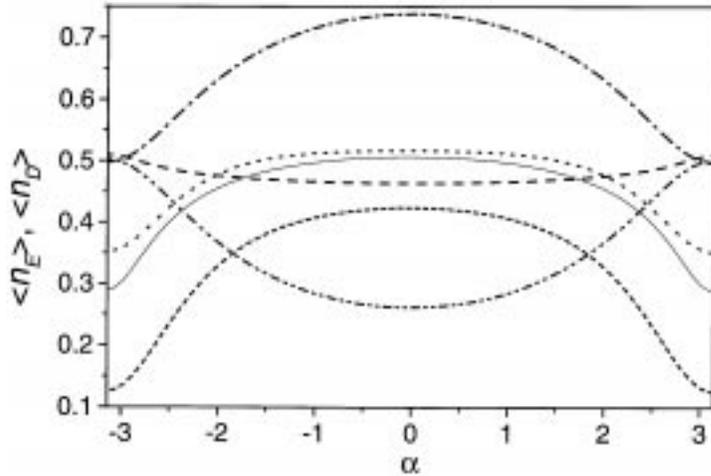
In figure 8, we plot $\langle n_D \rangle$ (dotted curve) and $\langle n_E \rangle$ (short-dashed curve), when $u/t = 0$, for the two-electron system. We then consider a situation when u is small and charge transfer between the ring and the stub is not important. When $u/t = 1$, then $\langle n_D \rangle$ is given by the thin solid curve while $\langle n_E \rangle$ is given by the long-dashed curve. One can see that u has decreased $\langle n_D \rangle$ and enhanced $\langle n_E \rangle$ thereby distributing the electrons evenly between the two sites.

That is a repulsive interaction between nearest neighbors is enhancing the overlap rather than destroying the overlap between these two nearest neighbor sites. One can actually see that the solid curve and the dashed curve are equal to each other around $|\alpha^*|$, i.e., when the single particle states of the isolated ring and the isolated stub are degenerate to each other and result in a NSDN at that energy. Now let us consider a situation when u is very large and hence the stub and the ring has one electron each and there is absolutely no charge transfer between the stub and the ring. When $u/t = 100$, then $\langle n_D \rangle$ is given by the dash-dotted curve, while $\langle n_E \rangle$ is given by the dot-dot-dashed curve. For infinite u, when the NSDN is pushed to the extreme end of the zone boundary, i.e. $|\alpha^*| = \pi$, and one electron is completely localized in the stub, then at $|\alpha^*| = \pi$, once again $\langle n_D \rangle = \langle n_E \rangle$. For such large values of u, at small α it can be seen that the electron in the stub mostly reside at the site D as expected but not at $\alpha = \alpha^*$.

The reason is as follows: The NSDN costs a lot of energy, and if the system can get rid of this NSDN then it gains in energy. When interaction is increased, then the stub electron has two options. Firstly, it can mostly reside in the the site D in order to reduce the interaction energy, but this does not help it to remove the NSDN. The NSDN merely moves into the stub and resides at site E rather than the site C. The other option is that the electron in the stub resides equally in the sites E and D, and the NSDN is pushed above the Fermi energy and does not affect the energetics of the system. The interacting electrons can now be thought to be moving in an effective potential, and the single particle states of the effective potential are like the states of an isolated stub and an isolated ring, with one electron in each of them. But the effective potential is such that the electron in the ring and the electron in the stub are nowhere degenerate. The degeneracy is removed by the way in which u renormalized the real potential to give the effective potential. This renormalization, populates the two stub sites equally and raises the energy of the electron localized in the stub with respect to the electron localized in the ring, such that the stub electron and the ring electron are not degenerate at any flux. In the absence of the degeneracy, the NSDN also do not exist or rather becomes marginal as in this case. The NSDN can be pushed to the extreme zone boundary but cannot be pushed beyond that for the presence of a gap in the spectrum. However large u we choose we see some effect of the NSDN. But in a system with a continuous spectrum it would be possible to remove the NSDN completely.

Thus we find that repulsive interaction in the presence of NSDN can result in some features that are typically like that of the attractive interaction between electrons. In this respect one may recall the fact that in a BCS superconductor also electrons can exhibit an attractive interaction between each other. They interact via an effective potential that is actually negative. Whereas in the present case studied by us, there is no effective potential that is negative. The interacting system always has a free energy higher than that of the non-interacting system, in the presence as well as in the absence of the NSDN. However, in the presence of the NSDN, the qualitative behavior of electron correlation effects is like that of an attractive potential. It is seen in high T_c superconductors, that electrons form pairs while there is no trace of any attraction between them. So probably one should study the possibilities of NSDN in two dimensional lattices.

The system considered here (i.e., three sites in the ring, two sites in the stub and 2 electrons in the whole system) gives a very good picture of the competition between repulsive interaction between electrons and NSDN. In larger systems, where the electrons tend to have greater degrees of freedom, the charge transfer between the ring and the stub often hides the effect. Numerical calculation suggest that the effect is still present but it is often

difficult to draw a clear conclusion by isolating the effect. Of course, there are infinite possibilities of choosing the system parameters and it may be possible to find some regimes where charge transfer is negligible and at the same time it is possible to tune the NSDN to lie exactly at the Fermi surface. Also, we have not considered the electron spin in the present study. The conclusions of an effective attraction between repulsive electrons of the same spin can be drawn on the basis of the study here. This is essentially because inclusion of spin will not destroy the effective attraction between electrons with the same spin. Of course there may be additional effects of NSDN-created effective attraction or repulsion between electrons with opposite spins. We are looking at such possibilities at present. Besides, for large values of u/t, the stub can be occupied by only one electron with a given spin, a phenomenon known as Coulomb Blockade and we believe the effect mentioned here can be experimentally verified. One should look for polarization effects of relative parts within the stub connected to a ring. The focus of ref. [18] was to look for the polarization of the stub with respect to the ring. Or one can also take two quantum dots, one at the position of site E and connected to the ring on one side and to another dot on the other side, the second dot being located at the site D. In such a geometry, one can study the polarization of the two dots with respect to each other, which will show the effects of this NSDN induced effective attraction. Such a study will be reported in the future.

References

[1] P Singha Deo, *Phys. Rev.* **B53**, 15447 (1996)
[2] A J Leggett, in *Granular nano-electronics, NATO Advanced Studies Institute, Series B: Physics* edited by D K Ferry, J R Barker and C Jacoboni (Plenum, New York, 1991) vol. 251, p. 297
[3] E Tekman and P F Bagwell, *Phys. Rev.* **B48**, 2553 (1993)
    W Porod, Z Shao and C S Lent, *Phys. Rev.* **B48**, 8495 (1993)
[4] U Fano, *Phys. Rev.* **124**, 1866 (1961)
[5] P F Bagwell, *Phys. Rev.* **B41**, 10354 (1990)
[6] P Singha Deo, *Solid State Commun.* **107**, 69 (1998)
[7] A Yacoby *et al*, *Phys. Rev. Lett.* **74**, 4047 (1995)
[8] R Schuster *et al*, *Nature (London)* **385**, 417 (1997)
[9] G Cernicchiaro *et al*, *Phys. Rev. Lett.* **79**, 273 (1997)
[10] L Yeyati and M Büttiker, *Phys. Rev.* **B52**, R14360 (1995)
[11] P Singha Deo and A M Jayannavar, *Mod. Phys. Lett.* **B10**, 787 (1996)
[12] C-Mo Ryu and S Y Cho, *Phys. Rev.* **B58**, 3587 (1998)
[13] H Xu and W Sheng, *Phys. Rev.* **B57**, 11903 (1998)
[14] H W Lee, *Phys. Rev. Lett.* **82**, 2358 (1999)
[15] T Taniguchi and M Buttiker, *Phys. Rev.* **B60**, 13814 (1999)
[16] A L Yeyati and M Büttiker, cond-mat/0006281
[17] P Singha Deo, S Bandopadhaya and S Das, cond-mat/0102095
[18] M Büttiker, *Physi. Scr.* **T54**, 104, 1994
    M Büttiker and C A Stafford, *Phys. Rev. Lett.* **76**, 495 1996
    P Cedraschi and M Buttiker, *J. Phys. Condens. Matter* **10**, 3985 (1998)
[19] M Büttiker, Y Imry and R Landauer, *Phys. Lett.* **96A**, 365 (1983)
[20] P A Sreeram and P Singha Deo, *Physica* **B228**, 345 (1996)