5 Charge transport in the presence of electron-electron interactions

In this thesis so far we have explored quantum transport of spinless electrons in the absence of interactions or in the presence of effective interactions modeled phenomenologically via voltage probes. Now we embark on studying the effect of electron-electron Coulomb interactions on quantum charge transport from first principle. Here we are mostly interested in microscopic description of transport phenomena in mesoscopic low dimensional systems. We have developed an analytical approach based on Lippmann-Schwinger scattering theory to deal with non-equilibrium physics of the locally interacting electrons at zero temperature [173]. An understanding of the behavior of electrons interacting with each other in a localized region has been a challenging problem in theoretical physics. Recently, it has attracted much attention in view of the experimental interest in transport across quantum dots and the Kondo effect in a quantum dot [174–178]. Another important question is whether electron-electron interaction decoheres the system in the presence of finite bias even in zero temperature? There are also several other interesting phenomena that can be studied in the presence of interactions in mesoscopic systems at zero temperature, for example, interaction induced entanglement and resonances. Entanglement is the manifestation of quantum correlations between observable physical properties of two or more quantum subsystems even though individual systems may be spatially separated. As a prototypical model, let us consider two ideal leads (within which all electronic interactions can be neglected) connected to a region (a quantum dot) where the electrons interact. One is interested in the current through the dot in response to an applied voltage difference between the leads.

As has been discussed in Chapter (1), there are several different but equivalent theoretical approaches for solving this problem. In the nonequilibrium Green's function (NEGF) approach, the initial density matrix of the two reservoirs (taken as ideal Fermi liquids in equilibrium at different chemical potentials) and the dot (in an arbitrary initial state), is evolved in time. The coupling between the reservoirs and the dot is switched on adiabatically and one looks at the steady state properties of the resulting density matrix. A second approach is to view this as a time-independent scattering problem and to look for many-particle scattering states which have the correct asymptotic form in the leads. This second approach is in the spirit of the Landauer formalism. A third approach is to use the quantum Langevin equations method (LEGF), where

the reservoirs are treated as sources of noise and dissipation. In the case where there are no interactions in the dot region, exact results for the current and other steady state properties can be obtained, and all three approaches give identical answers [32, 179–181]. The interacting case however is much more difficult to study. For a single dot connected to noninteracting leads, some results using the NEGF method have been obtained using the so-called non-crossing approximation [181, 182]. For an integrable model, namely the interacting resonance level model, Mehta and Andrei were able to solve the problem exactly [29]. Using the Bethe ansatz [183], they were able to express all N-particle scattering states in terms of the two-particle S-matrix, which is known exactly. They considered a continuum model with a linear spectrum which makes it integrable. The N-particle scattering matrix for electrons interacting in a quantum dot has also been studied in Ref. [184].

In this chapter, we present the results of our study [173] of a lattice version of the model considered in Ref.[29]. In Sec.(5.1), we show that using the Lippmann-Schwinger method, all two-particle eigenstates of this model can be found $exactly$. The form of the S-matrix indicates that the model is not solvable by the Bethe ansatz. We examine the S-matrix and compare it with numerical experiments on scattering of a two-particle wave packet in Subsec.(5.1.2). We also study two-particle as well as many-body transport in this system in Sec.(5.2). We show that N-particle scattering states can be obtained easily within two particle scattering approximation for weak interactions. Using these, we obtain an expression for the change in the Landauer current across a dot arising from interactions. Here, we start with a very simplified model where we ignore on-site potentials of the dot and the coupling of the dot sites with the leads are also same as the other inter sites hopping. These assumptions physically mean that in the absence of interactions there is translational invariance in the model. Later, in Sec.(5.3), we discuss the more realistic models of transport through quantum dots. We note that the study of two-particle scattering states is in itself of interest [185, 186], apart from being the starting point for the study of many-particle states necessary to understand transport. Recently, Goorden and Büttiker [187, 188] have studied a set-up with two disconnected conducting wires and with electrons in the two wires interacting weakly in a localized region. Using first order perturbation theory, the two-particle S-matrix was evaluated and used to extract information on transmission and correlations in a two-particle scattering experiments. In our single channel case, we will show that the antisymmetry of the wave functions leads to striking asymmetries in the S-matrix. In another interesting recent work, the S-matrix in a model of two photons interacting with a localized atom was studied [189].

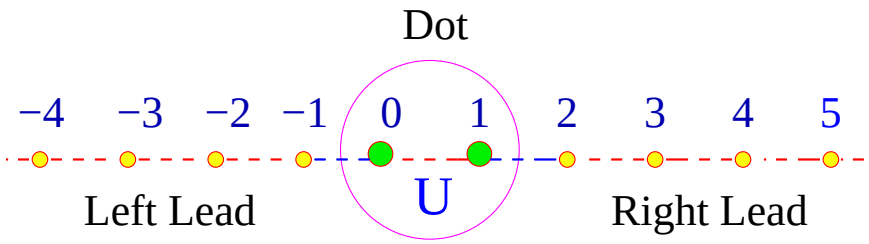

Figure 5.1: Schematic description of a single dot connected with two noninteracting leads

5.1 Model and exact two particle scattering states

We consider a tight-binding one-dimensional lattice with spinless electrons. The model considered describes an interacting dot on the sites $l = 0, 1$ (see Fig.(5.1)) which is connected to two noninteracting one-dimensional leads on either side. The Hamiltonian is given by

$$\begin{aligned} H &= H_L + H_D + V_C, \quad \text{where} \\ H_L &= -\sum_{l=-\infty}^{\infty}{}' \ (c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l), \\ H_D &= -(c_0^\dagger c_1 + c_1^\dagger c_0) + (\epsilon_0 n_0 + \epsilon_1 n_1) + U n_0 n_1 \\ \text{and } V_C &= -\gamma(c_{-1}^\dagger c_0 + c_0^\dagger c_{-1}) + \gamma'(c_1^\dagger c_2 + c_2^\dagger c_1), \end{aligned} \tag{5.1}$$

where $n_l = c_l^\dagger c_l$ is the number operator at site l, and $\sum'$ implies omission of $l = -1, 0, 1$ from the summation. We have set the hopping amplitude in the leads to be 1 and assume that the interaction is repulsive ($U > 0$); we also set the lattice spacing and $\hbar$ to be 1. First, we consider the couplings $\gamma = \gamma' = 1$ and on-site dot energies $\epsilon_0 = \epsilon_1 = 0$ corresponding (for $U = 0$) to the case of a perfectly transmitting dot.

5.1.1 Scattering states

We first show how one can obtain all the two-particle energy eigenstates exactly for this problem. Consider the noninteracting Hamiltonian $H_0 = H$ with $U = 0$. For this case, the one-particle eigenstates have the form $\phi_k(l) = e^{ikl}$ with energy $E_k = -2\cos k$, where $-\pi < k \leq \pi$. Now consider a two-particle incoming state given by $\phi_{\mathbf{k}}(\mathbf{l}) = e^{i(k_1 l_1 + k_2 l_2)} - e^{i(k_2 l_1 + k_1 l_2)}$, with $\mathbf{k} = (k_1, k_2)$ and $\mathbf{l} = (l_1, l_2)$. The energy of this state is $E_{\mathbf{k}} = E_{k_1} + E_{k_2}$. A scattering eigenstate $|\psi\rangle$ of H with energy E is related to a state $|\phi\rangle$ of H_0 through the Lippmann-Schwinger equation

$$\begin{aligned} |\psi\rangle &= |\phi\rangle + G_0^+(E) V |\psi\rangle, \\ \text{where } G_0^+(E) &= \frac{1}{E - H_0 + i\epsilon}. \end{aligned} \tag{5.2}$$

For the two-particle sector, in the position basis $|\mathbf{l}\rangle$ and with an incident state $< \mathbf{l}|\phi\rangle = \phi_{\mathbf{k}}(\mathbf{l})$, Eq. (5.2) gives

$$\begin{aligned} \psi_{\mathbf{k}}(\mathbf{l}) &= \phi_{\mathbf{k}}(\mathbf{l}) + UK_{E_{\mathbf{k}}}(\mathbf{l})\ \psi_{\mathbf{k}}(\mathbf{0}), \qquad (5.3) \\ \text{where}\ \ K_{E_{\mathbf{k}}}(\mathbf{l}) &= <\mathbf{l}|G_0^+(E_{\mathbf{k}})|\mathbf{0}\rangle, \end{aligned}$$

and $\mathbf{0} \equiv (1,0)$. We can determine $\psi_{\mathbf{k}}(\mathbf{0})$ using Eq. (5.3),

$$\psi_{\mathbf{k}}(\mathbf{0}) = \frac{\phi_{\mathbf{k}}(\mathbf{0})}{1 - UK_{E_{\mathbf{k}}}(\mathbf{0})}. \qquad (5.4)$$

The two-particle scattering eigenstate is completely given by Eqs. (5.3-5.4). The matrix elements $K_{E_{\mathbf{k}}}(\mathbf{l})$ are known explicitly and are given by

$$K_{E_{\mathbf{k}}}(\mathbf{l}) = g^+_{E_{\mathbf{k}}}(l_1 - 1, l_2) - g^+_{E_{\mathbf{k}}}(l_1, l_2 - 1), \qquad (5.5)$$

where $g^+_{E_{\mathbf{k}}}(\mathbf{l}) = [1/(2\pi)^2] \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} dq_1 dq_2 e^{i\mathbf{q}\cdot\mathbf{l}}/(\ E_{\mathbf{k}} - E_{\mathbf{q}} + i\epsilon)$ is the usual two-dimensional lattice Green's function. It is instructive to look at the asymptotic form of the scattered wave function [190]; this can be obtained by the saddle point method, the contribution to the integral in Eq. (5.5) coming from the region near $E_{\mathbf{q}} = E_{\mathbf{k}}$. Apart from a factor $U\psi_{\mathbf{k}}(\mathbf{0})$, we find asymptotically that

$$\begin{aligned} K^{as}_{E_{\mathbf{k}}}(\mathbf{l}) &= \frac{(\pm 1 - i)}{4\pi^{1/2}} \frac{e^{i(l_1 k_1' + l_2 k_2')}}{(r/r_0)^{1/2}} (e^{-ik_1'} - e^{-ik_2'}), \qquad (5.6) \\ \text{with}\ \ \frac{l_1}{\sin(k_1')} &= \frac{l_2}{\sin(k_2')}, \quad \text{where}\ \ l_i/\sin(k_i') > 0, \qquad (5.7) \\ E_{\mathbf{k}} &= -2\cos(k_1') - 2\cos(k_2'), \qquad (5.8) \\ r &= (l_1^2 + l_2^2)^{1/2}, \qquad (5.9) \\ \text{and}\ \ r_0 &= \frac{[\sin^2(k_1') + \sin^2(k_2')]^{1/2}}{|\sin^2(k_1')\cos(k_2') + \sin^2(k_2')\cos(k_1')|}, \end{aligned}$$

where the $\pm$ sign in Eq. (5.6) corresponds to $E_{\mathbf{k}}0$. The antisymmetry of the wave function is implicitly hidden in the $\mathbf{l}$-dependence of $\mathbf{k}'$. [The expression in Eq. (5.6) is clearly more complicated than the Bethe ansatz would have given which is a superposition of only four pairs of momenta, namely, $(\pm k_1, \pm k_2)$.] The physical interpretation of the above solution is as follows. Two electrons with initial momenta (k_1, k_2) emerge, after scattering, with momenta (k_1', k_2'). Energy is conserved as implied by Eq. (5.8), but the presence of interaction breaks the translational invariance, i.e., the total momentum is not conserved. The velocities of the electrons are given by $v_1 = 2\sin(k_1')$ and $v_2 = 2\sin(k_2')$; Eq. (5.7) expresses the fact that the electrons observed at (l_1, l_2) must reach there at the same time after collision. Note that we can equivalently think

of this problem as that of a single electron in a two-dimensional ($2D$) lattice moving in the half-space $l_1 > l_2$, with a hard wall along the diagonal $l_1 = l_2$ and a single impurity at the site $\mathbf{0}$. The particle flux $\vec{J}\cdot d\vec{S}$ in a given direction $tan(\theta) = l_2/l_1$ in the $2D$ problem corresponds, in the $1D$ problem, to the rate at which two particles are scattered with velocity ratio $v_2/v_1 = tan(\theta)$. Instead of the usual scattering cross-section, it is useful here to calculate the scattering rate for *unit two-particle density at the site* $\mathbf{0}$. This is given by

$$|f(\theta)|^2\ d\theta = \frac{\vec{J}\cdot d\vec{S}}{|\phi_{\mathbf{k}}(\mathbf{0})|^2} = \frac{1}{|1/U - K_{E_{\mathbf{k}}}(\mathbf{0})|^2}\frac{[1-\cos(k_1'-k_2')]\ [\sin^2(k_1')+\sin^2(k_2')]}{2\pi|\sin^2(k_1')\cos(k_2')+\sin^2(k_2')\cos(k_1')|}\ d\theta, \quad (5.10)$$

where k_1', k_2' are known in terms of θ. Note that the only dependence on the interaction parameter U is through the factor $|1/U - K_{E_{\mathbf{k}}}(\mathbf{0})|^2$. In an experiment, it may be simpler to find the number of particles scattering within an energy interval $dE_{k_2'}$ (energy conservation implies that $dE_{k_1'} + dE_{k_2'} = 0$). Defining $P(E_{k_1}, E_{k_2} \to E_{k_1'}, E_{k_2'})dE_{k_2'} = |\phi_{\mathbf{k}}(\mathbf{0})|^2|f(\theta)|^2 d\theta$, we find that

$$P(E_{k_1}, E_{k_2} \to E_{k_1'}, E_{k_2'}) = \frac{1-\cos(k_1-k_2)}{|1/U - K_{E_{\mathbf{k}}}(\mathbf{0})|^2}\ \frac{1-\cos(k_1'-k_2')}{4\pi|\sin(k_1')\sin(k_2')|}. \quad (5.11)$$

Finally, we can write an exact expression for the usual S-matrix,

$$S(\mathbf{k},\mathbf{k}') \ = \ -\ \frac{i\pi(e^{ik_1}-e^{ik_2})(e^{-ik_1'}-e^{-ik_2'})}{1/U - K_{E_{\mathbf{k}}}(\mathbf{0})}. \quad (5.12)$$

5.1.2 Time evolution of two-particle wave packets

For the two-particle case it is more useful to study wave packets. We now consider the time evolution of wave packets and see how well the predictions of the scattering theory hold. The scattering states given by Eq. (5.3) are the full set of allowed two-particle energy eigenstates (for $U > \pi$ one gets an additional bound state). These can be generated by a unitary time evolution of the unperturbed states which form a complete set. Hence these states also form a complete set, and any two-particle wave function can be expanded using this basis. Thus the time evolution of an initial wave packet $\Psi(\mathbf{l}, t=0)$ is given by

$$\Psi(\mathbf{l},t) = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} dq_1 \int_{-\pi}^{q_1} dq_2\ a(\mathbf{q})\psi_{\mathbf{q}}(\mathbf{l})\ e^{-iE_{\mathbf{q}}t},$$
$$\text{where}\ \ a(\mathbf{q}) = \sum_{l_1>l_2} \Psi(\mathbf{l},t=0)\ \psi^*_{\mathbf{q}}(\mathbf{l}). \quad (5.13)$$

The time evolution can be studied quite accurately because of our knowledge of the exact basis states. In evaluating the basis states, for small $(l_1, l_2) \leq 15$, we evaluate the necessary Green's functions $g^+_{E_{\mathbf{k}}}(\mathbf{l})$ exactly using recursion relations relating these to $g^+_{E_{\mathbf{k}}}(0,0)$ and $g^+_{E_{\mathbf{k}}}(1,1)$. For larger (l_1, l_2) we use the asymptotic forms which are quite accurate. We find that in our computations the normalization of the wave function is preserved to within 0.5%. In Fig.(5.2) we

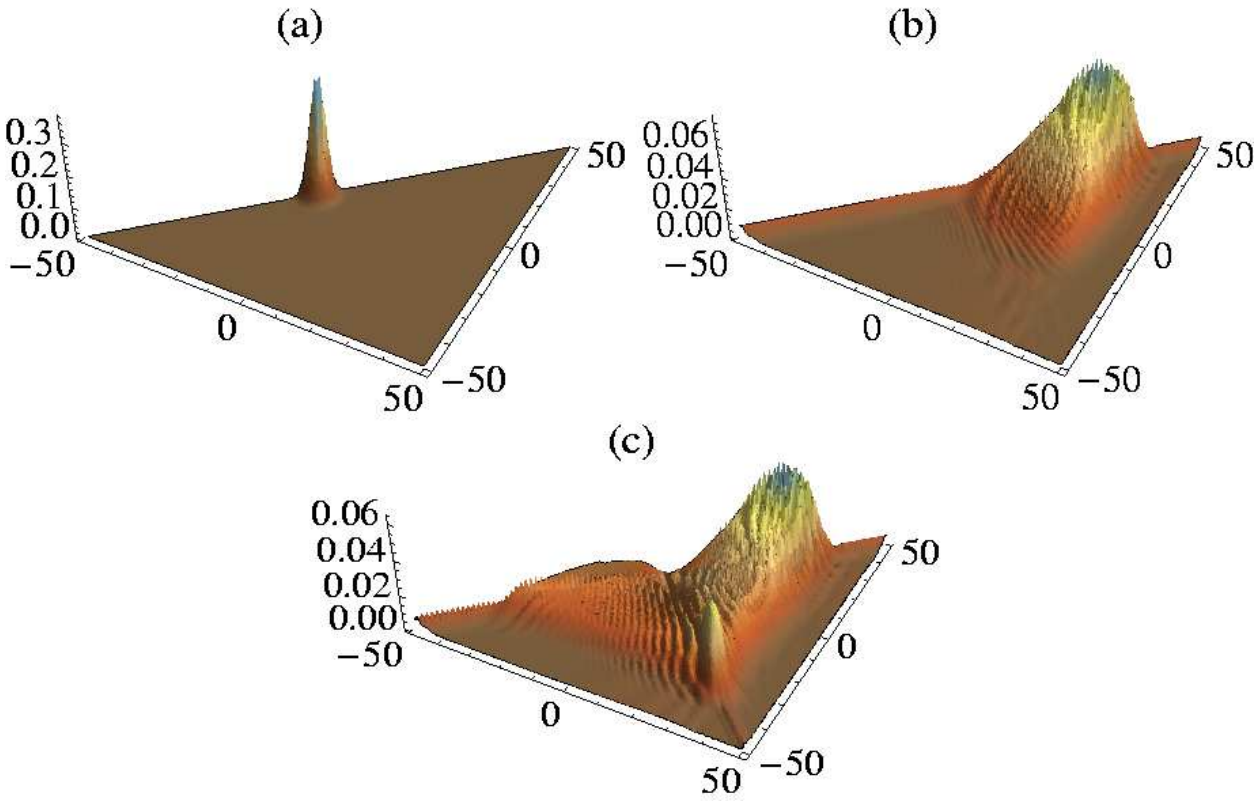

FIGURE 5.2: Plot of the evolution of an incident wave packet (a) after passing through the origin with $U = 0$ in (b) and $U = 2$ in (c). Note the strong scattering at an angle $\theta = -\pi/4$.

show the typical time-evolution of a wave packet with initial position and momentum localized at $\mathbf{l} = (-5, -6.8)$ and $\mathbf{q} = (2.36, 1.87)$ respectively and with widths $\delta l \approx \delta q \approx 1$ and $E \approx 0$. These initial conditions have been chosen so that the two particles reach the site $\mathbf{0}$ at roughly the same time; this maximizes their interaction. The initial wave packet shown in Fig.(5.2(a)) evolves at time $t = 20$ to (b) for $U = 0$ and to (c) for $U = 2$. For the scattered wave function in Fig.(5.2 (c)) we can count the number of particles scattered into a given direction. This is plotted in Fig.(5.3) for incident wave packets with different energies. We also compare this with the scattering theory prediction by plotting $|f(\theta)|^2$ multiplied by the time-integrated incident two-particle density at the origin. The comparison can be seen to be very good.

5.1.3 Bound states:

For $|E| > 4$, the imaginary part of $K_E(\mathbf{0})$ vanishes; hence a localized state at a discrete energy level E_b can occur under the condition

$$1 \; - \; UK_{E_b}(\mathbf{0}) \; = \; 0. \tag{5.14}$$

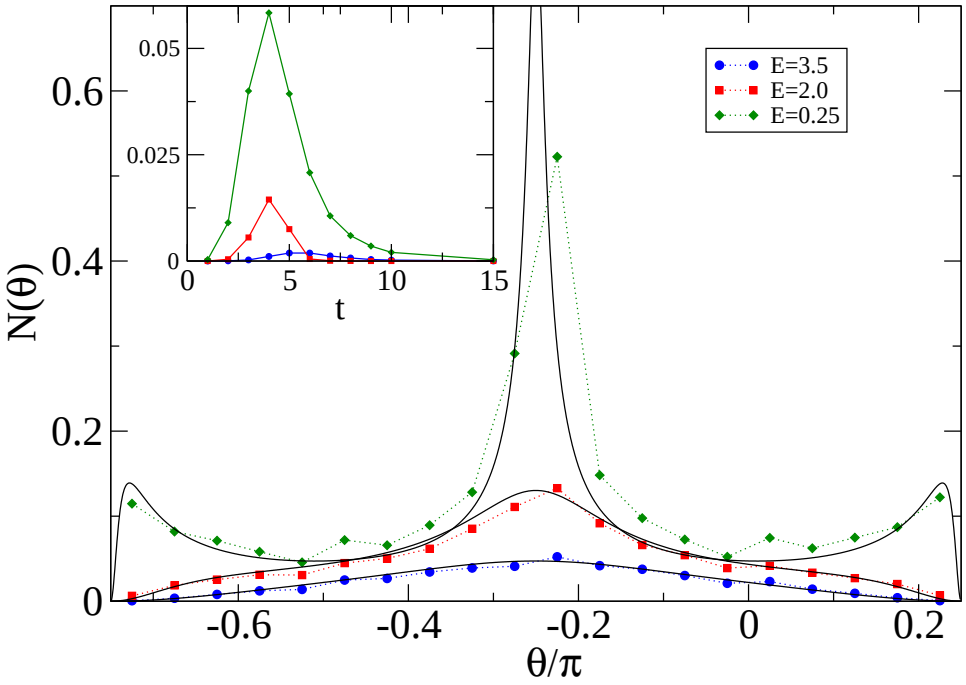

FIGURE 5.3: Plot of the number of particles scattered into a given direction for incident wave packets with different energies. The bold lines show the results from scattering theory estimated using $|f(\theta)|^2$ and the incident particle density at the origin (inset). Inset shows $|\Psi_{inc}(\mathbf{0},t)|^2$.

This equation can be solved to give E_b as a function of the interaction strength U. The minimum energy for a (positive energy) bound state is $E_b = 4$; Eq. (5.14) then leads to the condition $U > \pi$. It is easy to show that this discrete level is in fact a localized state, i.e., it has a normalizable wave function which decays exponentially when the coordinate of either particle goes to $\pm\infty$. To prove this we note that for $E_b > 4$, the two-particle eigenstate obeys the equation $|\psi\rangle = [1/(E_b - H_0)]\ V\ |\psi\rangle$. This enables us to write the wave function at any point $\mathbf{l}$ in terms of its value at $\mathbf{0}$. Thus $\psi(\mathbf{l}) = K_{E_b}(\mathbf{l})U\psi(\mathbf{0})$. Now it is known [190] that for E_b lying outside the bandwidth of the leads $[-2,2]$, $g^+_{E_b}(\mathbf{l})$ and hence $K_{E_b}(\mathbf{l})$ decay exponentially with $|\mathbf{l}|$. This proves that $\psi(\mathbf{l})$ is a normalizable bound state.

5.2 Transport calculation:

5.2.1 Two-particle sector

We will now turn our attention to quantities of interest in transport calculations. The current density is given by the expectation value of the operator $j_l = -i(c_l^\dagger c_{l+1} - h.c.)$ in the scattering

state $|\psi_{\mathbf{k}}\rangle = |\phi_{\mathbf{k}}\rangle + |S_{\mathbf{k}}\rangle$. The current in the incident state is given by

$$\langle\phi_{\mathbf{k}}|j_l|\phi_{\mathbf{k}}\rangle = 2[\sin(k_1) + \sin(k_2)]\mathcal{N}, \tag{5.15}$$

where $\mathcal{N}$ is a normaliation constant depicting the total number of sites in the entire system. The change in current due to repulsive interactions has contributions from two parts given by,

$$\begin{aligned}\delta j(k_1, k_2) &= \langle\psi_{\mathbf{k}}|j_l|\psi_{\mathbf{k}}\rangle - \langle\phi_{\mathbf{k}}|j_l|\phi_{\mathbf{k}}\rangle, \\ &= \langle S_{\mathbf{k}}|j_l|S_{\mathbf{k}}\rangle + \langle S_{\mathbf{k}}|j_l|\phi_{\mathbf{k}}\rangle + \langle\phi_{\mathbf{k}}|j_l|S_{\mathbf{k}}\rangle \end{aligned} \tag{5.16}$$

We evaluate them separately in the different sides of the interating region. For the first part (call auto-correlation) we find for $k_1, k_2 > 0$,

$$j_S = \langle S_{\mathbf{k}}|j_l|S_{\mathbf{k}}\rangle = \frac{1}{\pi}\frac{|\phi_{\mathbf{k}}(\mathbf{0})|^2}{|1/U - K_{E_{\mathbf{k}}}(\mathbf{0})|^2}\int_{\cos^{-1}(1-E_{\mathbf{k}}/2)}^{\pi} dp_1 \frac{1-\cos(p1)\cos q}{\sin q} \tag{5.17}$$

for $l > 1$ and with a negative sign for the region $l < 0$. Here $E_{\mathbf{k}} - E_{p_1} = -2\cos q$ with $q > 0$. Similarly we calculate the cross-contribution in the current and this is given by

$$j_C = \langle S_{\mathbf{k}}|j_l|\phi_{\mathbf{k}}\rangle + \langle\phi_{\mathbf{k}}|j_l|S_{\mathbf{k}}\rangle = \frac{-2i|\phi_{\mathbf{k}}(\mathbf{0})|^2}{1/U - K_{E_{\mathbf{k}}}(\mathbf{0})|^2}[K_{E_{\mathbf{k}}}(\mathbf{0}) - K^*_{E_{\mathbf{k}}}(\mathbf{0})]. \tag{5.18}$$

Both j_S and j_C is of order 1, i.e., it is a factor of $\mathcal{N}$ smaller than the current in the incident state [186]. After summing up both the contributions in the left and right side of the dot separately, we determine total change in the current due to scattering which is same in the both sides as should be for current conservation.

$$\delta j(k_1, k_2) = \frac{2|\phi_{\mathbf{k}}(\mathbf{0})|^2 Im[K_{E_{\mathbf{k}}}(\mathbf{0})]}{|1/U - K_{E_{\mathbf{k}}}(\mathbf{0})|^2}\ [sgn(k_1) + sgn(k_2)], \tag{5.19}$$

where $sgn(k) \equiv |k|/k$. One interesting point to notice here that the first order change in the current is quadratic in interactions for the dot without on-site energies. Later we will see that in the case of more generalised dot where on-site energies due to applied gate voltage is included, the first order change in the current is linear in interactions strength U.

5.2.2 N-particle scattering states and change in the Landauer current

We now consider the problem of calculating the current in a situation where the interacting region is connected to left and right leads which are at zero temperature and chemical potentials μ_L and μ_R respectively. In that case we need to consider an initial state with N_L electrons in positive momentum states filling 1-particle energy levels up to μ_L and N_R electrons in negative momentum states filling levels up to μ_R. Let $N = N_L + N_R$ and let us denote this N-particle incident wave by $|\phi^{(N)}\rangle = |\mathbf{k}^{(N)}\rangle$, where $\mathbf{k}^{(N)} = \{k_1 k_2 ... k_N\}$. One then needs to find the corresponding scattering

state and compute the particle current. While an exact solution for the N-particle scattering state looks difficult, it is straight-forward to obtain a perturbative solution at first order in U. The scattered wave is given by $|\psi_{\mathbf{k}_N}\rangle = |\phi_{\mathbf{k}_N}\rangle + |S_{\mathbf{k}_N}\rangle$ with $|S_{\mathbf{k}_N}\rangle = G_0^+ V|\mathbf{k}_N\rangle$. At order U, the transition amplitude to a wave vector $\mathbf{q}_N = \{q_1 q_2 ... q_N\}$ can be expressed in terms of the two-particle transitions. Thus

$$\begin{aligned} \langle \mathbf{q}_N | S_{\mathbf{k}_N} \rangle &= \sum_{\mathbf{q}_2 \mathbf{k}_2} (-1)^{P+P'} \langle \mathbf{q}_2 | S_{\mathbf{k}_2} \rangle \langle \mathbf{q}'_{N-2} | \mathbf{k}'_{N-2} \rangle, \\ \text{where } \langle \mathbf{q}_2 | S_{\mathbf{k}_2} \rangle &= \frac{U \phi^*_{\mathbf{q}_2}(\mathbf{0}) \phi_{\mathbf{k}_2}(\mathbf{0})}{E_{\mathbf{k}} - E_{\mathbf{q}} + i\epsilon} \end{aligned} \tag{5.20}$$

is the two-particle transition amplitude at order U, $\mathbf{q}_2$ ($\mathbf{k}_2$) denotes a pair of momenta chosen from the set $\mathbf{q}_N$ ($\mathbf{k}_N$), and $\mathbf{q}'$ ($\mathbf{k}'$) denotes the remaining $N-2$ momenta. P (P') are the appropriate number of permutations. Using Eq. (5.20), we calculate the current expectation value for the state $|\psi_{\mathbf{k}_N}\rangle$. The current in the incident state $|\phi_{\mathbf{k}_N}\rangle$ is given by $\langle \phi | j_l | \phi \rangle = 2[\sum_{j=1}^{N} \sin(k_j)] \mathcal{N}^{N-1}$. The correct normalization is obtained by dividing by a factor $\mathcal{N}^N$ which then gives in the continuum limit:

$$\begin{aligned} j_{inc} &= \frac{1}{2\pi} \left[\int_0^{k_L} dk \; 2\sin(k) - \int_0^{k_R} dk \; 2\sin(k) \right] \\ &= \frac{1}{2\pi} \; (\mu_L - \mu_R), \end{aligned} \tag{5.21}$$

where $k_{L,R} = \cos^{-1}(-\mu_{L,R}/2)$, and we have used $dk = dE/|dE/dk| = dE/|2\sin(k)|$. Inserting factors of $\hbar$ and e, Eq. (5.21) gives the expected Landauer current $I = (e/h)(\mu_L - \mu_R)$ and Landauer conductance $G = e^2/h$. The change in the Landauer current due to the scattering involves a rather long calculation but the final answer is simple. Surprisingly, we find that it can be expressed as a sum of two-particle currents from all possible momentum pairs: $\delta j_N = (1/2) \sum_{r,s} \delta j(k_r, k_s) \; \mathcal{N}^{N-2}$ which, with the same normalization as used earlier, gives

$$\delta j_N = \frac{1}{2(2\pi)^2} \int \int dk_1 dk_2 \; \delta j(k_1, k_2), \tag{5.22}$$

where the integrations are over the full range of allowed momenta in $\mathbf{k}_N$, and $\delta j(k_1, k_2)$ is given by Eq. (5.19) [expanded to order U^2]. Using the fact that $\delta j(k_1, k_2)$ vanish whenever k_1, k_2 have opposite signs and converting Eq. (5.22) to energy integrals, we finally get the following correction to the Landauer current:

$$\begin{aligned} \delta j_N &= \left[\int_{-2}^{\mu_R} dE_{k_1} \int_{\mu_R}^{\mu_L} dE_{k_2} + \frac{1}{2} \int_{\mu_R}^{\mu_L} dE_{k_1} \int_{\mu_R}^{\mu_L} dE_{k_2} \right] \\ &\times \; \rho(E_{k_1}) \rho(E_{k_2}) \; U^2 4 |\phi_{k_1,k_2}(\mathbf{0})|^2 \; Im[K_{E_{k_1,k_2}}(\mathbf{0})], \end{aligned} \tag{5.23}$$

where $\rho(E) = 1/(2\pi\sqrt{4 - E^2})$ is the density of states. The quantity in Eq. (5.23) is negative because $Im[K_{E_{\mathbf{k}}}(\mathbf{0})] < 0$ for all values of $\mathbf{k}$. In the zero bias limit $\mu_L \to \mu_R$, the expression in

(5.23) vanishes as $U^2(\mu_L - \mu_R)$ due to the contribution coming from the first set of integrals; thus the conductance is less than e^2/h by a term of order U^2.

It may seem surprising that although the two-particle scattering depends on a fine tuning of the initial conditions so that the particles arrive at the site $\mathbf{0}$ at the same time, the correction to the current from the scattering given in Eq. (5.23) requires no such fine tuning. This is because in the presence of a Fermi sea, the densities at the sites 0 and 1 are non-zero at all times. This can be seen by using the Hartree-Fock approximation to expand $Uc_0^\dagger c_0 c_1^\dagger c_1 = U[< c_0^\dagger c_0 > c_1^\dagger c_1 + < c_1^\dagger c_1 > c_0^\dagger c_0 - < c_1^\dagger c_0 > c_0^\dagger c_1 - < c_0^\dagger c_1 > c_1^\dagger c_0]$. If the Fermi sea is one in which all momenta lying in the range $-k_F < k < k_F$ are occupied (where $0 < k_F < \pi$), we obtain $< c_0^\dagger c_0 > = < c_1^\dagger c_1 > = k_F/\pi$, while $< c_1^\dagger c_0 > = < c_0^\dagger c_1 > = \sin(k_F)/\pi$. The problem then reduces to that of a single particle moving in the presence of a localized inhomogeneity in the on-site potential and in the hopping [191]; the strength of both of these is proportional to U. We can solve this one-particle problem to obtain a transmission probability $T(E)$ which is a function of the particle energy E; to lowest order, $T(E)$ is equal to 1 minus a term of order U^2. The Landauer formula for the current is given by $(e/2\pi)\int_{\mu_R}^{\mu_L} dE T(E)$; in the zero bias limit, the reduction in the current is therefore of the order of $U^2(\mu_L - \mu_R)$.

5.3 Generalization to realistic dot Hamiltonians:

In this section, we discuss the more realistic model of quantum dots and how exact two-particle eigenstates can be found for this case, i.e., arbitrary values of the parameters $\gamma, \gamma', \epsilon_0, \epsilon_1$ in Eq. (5.1) [192]. Again in this section we confine our discussions to spinless electrons. We begin by setting the interaction $U = 0$. The one-particle eigenstates of Eq. (5.1) can be found exactly, since it has a quadratic form. For a particle coming from the left, the complete wave function is given by

$$\begin{aligned} \phi_k(l) &= e^{ikl} + r_k e^{-ikl} \text{ for } l \leq -1, \\ &= (1 + r_k)/\gamma \text{ for } l = 0, \text{ and } t_k e^{ik}/\gamma' \text{ for } l = 1, \\ &= t_k e^{ikl} \text{ for } l \geq 2, \end{aligned} \tag{5.24}$$

where $0 < k < \pi$. Similarly, for a particle coming from the right, the wave function is given by

$$\begin{aligned} \phi_k(l) &= t_k e^{ikl} \text{ for } l \leq -1, \\ &= t_k/\gamma \text{ for } l = 0, \text{and } (e^{ik} + r_k e^{-ik})/\gamma' \text{ for } l = 1, \\ &= e^{ikl} + r_k e^{-ikl} \text{ for } l \geq 2, \end{aligned} \tag{5.25}$$

where $-\pi < k < 0$. The transmission (reflection) amplitudes t_k (r_k) can be found by solving the one-particle Schrödinger equation,

$$\begin{aligned} t_k &= \frac{-2i\gamma\gamma' e^{-ik}\sin k}{(\epsilon_1-\epsilon_k-\gamma'^2 e^{ik})(\epsilon_0-\epsilon_k-\gamma^2 e^{ik})-1}\ , \\ r_k &= \frac{1-(\epsilon_1-\epsilon_k-\gamma'^2 e^{ik})(\epsilon_0-\epsilon_k-\gamma^2 e^{-ik})}{(\epsilon_1-\epsilon_k-\gamma'^2 e^{ik})(\epsilon_0-\epsilon_k-\gamma^2 e^{ik})-1}. \end{aligned} \tag{5.26}$$

for $0 < k < \pi$, and for $-\pi < k < 0$

$$\begin{aligned} t_k &= \frac{2i\gamma\gamma' e^{ik}\sin k}{(\epsilon_1-\epsilon_k-\gamma'^2 e^{-ik})(\epsilon_0-\epsilon_k-\gamma^2 e^{-ik})-1}\ , \\ r_k &= \frac{e^{2ik}[1-(\epsilon_1-\epsilon_k-\gamma'^2 e^{ik})(\epsilon_0-\epsilon_k-\gamma^2 e^{-ik})]}{(\epsilon_1-\epsilon_k-\gamma'^2 e^{-ik})(\epsilon_0-\epsilon_k-\gamma^2 e^{-ik})-1}. \end{aligned} \tag{5.27}$$

A two-particle incoming state with momenta (k_1, k_2) has the wave function $\phi_{\mathbf{k}}(\mathbf{l}) = \phi_{k_1}(l_1)\phi_{k_2}(l_2) - \phi_{k_1}(l_2)\phi_{k_2}(l_1)$; the total energy is $E_{\mathbf{k}} = -2\cos(k_1) - 2\cos(k_2)$ as before. We now find the scattering eigenstate $\psi_{\mathbf{k}}$ using the same arguments as in Eqs. (5.2-5.4), except that $K_{E_{\mathbf{k}}}(\mathbf{l})$ is now given by

$$K_{E_{\mathbf{k}}}(\mathbf{l}) = \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{dq_1 dq_2}{(2\pi)^2}\ \frac{1}{E_{\mathbf{k}} - E_{\mathbf{q}} + i\epsilon}\phi_{q_1}(l_1)\phi_{q_2}(l_2)[\phi^*_{q_1}(1)\phi^*_{q_2}(0) - \phi^*_{q_1}(0)\phi^*_{q_2}(1)]. \tag{5.28}$$

We are assuming that there are no one-particle bound states; otherwise $K_{E_{\mathbf{k}}}(\mathbf{l})$ will receive a contribution from such states also. We can obtain the scattered wave function by looking at the asymptotic form of $K_{E_{\mathbf{k}}}(\mathbf{l})$ for large $|\mathbf{l}|$. The contribution to the integral in Eq. (5.28) comes from the region near $E_{\mathbf{q}} = E_{\mathbf{k}}$, due to the presence of the reflection amplitude r_k, and one will obtain contributions from four points $(\pm q_1, \pm q_2)$.

The above analysis for a general dot can be used to study some interesting problems. For instance, one can study resonant transmission of two particles through the dot assisted by the interactions between them. Suppose that the one-particle Hamiltonian has a form such that there are two one-particle energies E_{r1} and E_{r2} at which a particle can transmit though the dot, but it cannot transmit if its energy is different from $E_{r1},\ E_{r2}$. Now imagine sending in two particles whose energies $E_1,\ E_2$ are not at resonance but $E_1 + E_2 = E_{r1} + E_{r2}$. Then the interaction in the dot allows the two particles to make a transition from $E_1,\ E_2$ to $E_{r1},\ E_{r2}$ and thereby transmit through the dot. [The situation is somewhat reminiscent of Ref. [189] where it is shown that two photons can transmit together through a region in which they interact with each other.] Another application of the general dot analysis would be to consider a case in which the one-particle Hamiltonian has a bound state, and study how this state evolves as the strength of the interaction is varied [185].

Transport calculation: Now, we evaluate the two-particle current through a dot with some on-site energies. Again, we are interested in calculating the expectation value of the current

operator j_l, as defined in sec.(5.2), in the two-particle scattering state $|\psi_{\mathbf{k}}\rangle = |\phi_{\mathbf{k}}\rangle + |S_{\mathbf{k}}\rangle$. We assume that both the particles are incoming from left, i.e., $k_1, k_2 > 0$. First, we determine the current in the absence of interactions.

$$j_I = 2\ \mathrm{Im}[\langle\phi_{\mathbf{k}}|c_l^\dagger c_{l+1}|\phi_{\mathbf{k}}\rangle]. \tag{5.29}$$

$$\begin{aligned}
\langle\phi_{\mathbf{k}}|c_l^\dagger c_{l+1}|\phi_{\mathbf{k}}\rangle &= \sum_{mnm'n'} \frac{1}{2^2}\langle\phi_{\mathbf{k}}|mn\rangle\langle mn|c_l^\dagger c_{l+1}|m'n'\rangle\langle m'n'|\phi_{\mathbf{k}}\rangle \\
&= \sum_{mnm'n'} \frac{1}{2^2}\langle\phi_{\mathbf{k}}|mn\rangle\langle 0|c_n c_m c_l^\dagger c_{l+1} c_{m'}^\dagger c_{n'}^\dagger|0\rangle\langle m'n'|\phi_{\mathbf{k}}\rangle \\
&= \sum_m \frac{1}{2^2}\big(\langle\phi_{\mathbf{k}}|m,l\rangle\langle m,l+1|\phi_{\mathbf{k}}\rangle + \langle\phi_{\mathbf{k}}|l,m\rangle\langle l+1,m|\phi_{\mathbf{k}}\rangle \\
&\qquad - \langle\phi_{\mathbf{k}}|m,l\rangle\langle l+1,m|\phi_{\mathbf{k}}\rangle - \langle\phi_{\mathbf{k}}|l,m\rangle\langle m,l+1|\phi_{\mathbf{k}}\rangle\big) \\
&= \sum_m \langle\phi_{\mathbf{k}}|m,l\rangle\langle m,l+1|\phi_{\mathbf{k}}\rangle \\
&= \mathcal{N}\ (\phi_{k_2}^*(l)\phi_{k_2}(l+1) + \phi_{k_1}^*(l)\phi_{k_1}(l+1)).
\end{aligned} \tag{5.30}$$

So, the current in the noninteracting case is given by

$$j_I \ = \ 2\mathcal{N}\ (|t_{k1}|^2 \sin k_1 + |t_{k2}|^2 \sin k_2). \tag{5.31}$$

Next, we calculate the contribution to $\langle j\rangle$ from only the scattered part of the full wave function. This is given by

$$j_S \ = \ 2\ \mathrm{Im}[\langle S_{\mathbf{k}}|c_l^\dagger c_{l+1}|S_{\mathbf{k}}\rangle]. \tag{5.32}$$

$$\begin{aligned}
\langle S_{\mathbf{k}}|c_l^\dagger c_{l+1}|S_{\mathbf{k}}\rangle &= \sum_m \langle S_{\mathbf{k}}|m,l\rangle\langle m,l+1|S_{\mathbf{k}}\rangle \\
&= \frac{|\phi_{\mathbf{k}}(\mathbf{0})|^2}{|1/U - K_{E_{\mathbf{k}}}(\mathbf{0})|^2} \sum_m \langle\mathbf{0}|G_0^-(E_{\mathbf{k}})|m,l\rangle\langle m,l+1|G_0^+(E_{\mathbf{k}})|\mathbf{0}\rangle \\
&= \frac{|\phi_{\mathbf{k}}(\mathbf{0})|^2}{|1/U - K_{E_{\mathbf{k}}}(\mathbf{0})|^2} \int_{-\pi}^{\pi} \frac{dq_1}{2\pi}\ I_1(q_1) I_2(q_1), \\
\text{where}\ \ I_1 &= \int_{-\pi}^{\pi} \frac{dq_2}{2\pi}\ \frac{\phi_{q_1 q_2}(\mathbf{0})}{E_{\mathbf{k}} - E_{q_1 q_2} - i\epsilon}\ \phi_{q_2}^*(l), \\
I_2 &= \int_{-\pi}^{\pi} \frac{dq_4}{2\pi}\ \frac{\phi_{q_1 q_4}^*(\mathbf{0})}{E_{\mathbf{k}} - E_{q_1 q_4} + i\epsilon}\ \phi_{q_4}(l+1).
\end{aligned} \tag{5.33}$$

Finally, we evaluate the cross contribution to the current from the incident and scattered parts, given by

$$j_C \ = \ 2\ \mathrm{Im}[\langle\phi_{\mathbf{k}}|(c_l^\dagger c_{l+1} - c_{l+1}^\dagger c_l)|S_{\mathbf{k}}\rangle]. \tag{5.34}$$

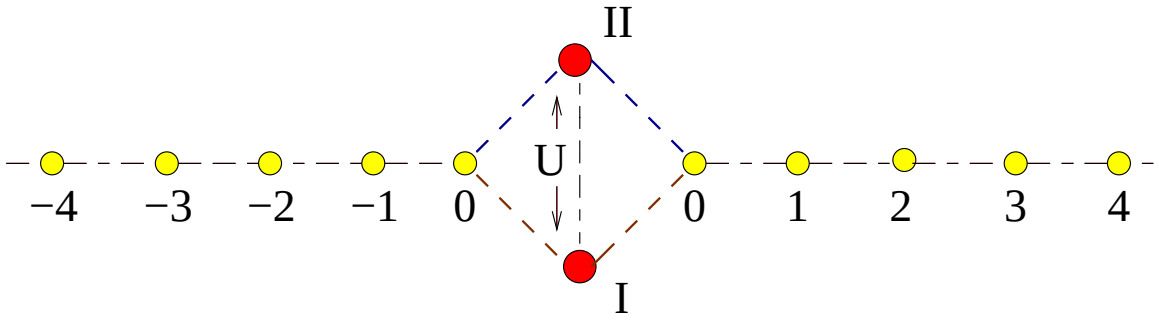

Figure 5.4: Schematic illustration of the coupled parallel double- dots with on-site dot potentials

We calculate the first term of the expression in Eq. (5.34).

$$\begin{aligned}\langle\phi_{\mathbf{k}}|c_l^\dagger c_{l+1}|S_{\mathbf{k}}\rangle &= \sum_m \langle\phi_{\mathbf{k}}|m,l\rangle\langle m,l+1|S_{\mathbf{k}}\rangle \\ &= \frac{\phi_{\mathbf{k}}(\mathbf{0})}{1/U - K_{E_{\mathbf{k}}}(\mathbf{0})} \sum_m \langle\phi_{\mathbf{k}}|m,l\rangle\langle m,l+1|G_0^+(E_{\mathbf{k}})|\mathbf{0}\rangle \\ &= \frac{\phi_{\mathbf{k}}(\mathbf{0})}{1/U - K_{E_{\mathbf{k}}}(\mathbf{0})} \int_{-\pi}^{\pi} \frac{dq_2}{2\pi}\Big(\frac{\phi^*_{k_2}(l)\phi_{q_2}(l+1)\phi^*_{k_1q_2}(\mathbf{0})}{E_{k_2}-E_{q_2}+i\epsilon} - \frac{\phi^*_{k_1}(l)\phi_{q_2}(l+1)\phi^*_{k_2q_2}(\mathbf{0})}{E_{k_1}-E_{q_2}+i\epsilon}\Big) \end{aligned} \quad (5.35)$$

Similarly, one can write the second term. For the simplified model of the dot, it has been possible to evaluate the above integrals in Eqs. (5.33, 5.35) explicitly and derive a closed form expression. Here, instead, we need to evaluate the integrals numerically to find the change in current due to interaction.

It is possible to employ the above method based on Lippmann-Schwinger scattering theory for several interesting relevant mesoscopic models. In this approach, as we have seen, one can calculate the two-particle current exactly and the current in the presence of Fermi sea in leads perturbatively. Transport through electrostatically coupled double-dots is another such example. Recently, double quantum dots set-up has got a lot of interest theoretically as well as experimentally in realizing quantum dot based quantum computations.

5.4 Scattering of spin $1/2$ electrons due to interactions

Finally, let us briefly discuss the case of spin-1/2 electrons. We consider the Hamiltonian

$$H = -\sum_{l=-\infty}^{\infty}\sum_{\sigma=\uparrow,\downarrow}(c^\dagger_{l,\sigma}c_{l+1,\sigma} + h.c.) + Un_{0\uparrow}n_{0\downarrow}. \quad (5.36)$$

The interaction at the site 0 can cause scattering between two electrons in the singlet channel but not in the triplet channel. This causes some sort of filtering for the spin-polarizations and generates entangled spin singlet in the reflected beams. The scattering of two electrons in

the singlet channel can be studied exactly using the Lippman-Schwinger formalism, just as in Eqs. (5.2-5.4), except that the wave function for the state $|\phi_{\mathbf{k}}\rangle \equiv |k_1,\uparrow;k_2,\downarrow\rangle = -|k_2,\downarrow;k_1,\uparrow\rangle$ is now given by $\phi_{\mathbf{k}}(\mathbf{l}) = e^{i(k_1 l_1 + k_2 l_2)}$, and the Green's function is given by $K_{E_{\mathbf{k}}}(\mathbf{l}) = [1/(2\pi)^2]\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} dq_1 dq_2 e^{i\mathbf{q}\cdot\mathbf{l}}/(\ E_{\mathbf{k}} - E_{\mathbf{q}} + i\epsilon)$. Finally, we can argue, as in the spinless case, that in the presence of a Fermi sea, the scattering reduces the Landauer conductance by a term of order U^2; the Hartree-Fock approximation also gives this result in a simple way. We note that the bound states for the two-particle problem in the spin-$1/2$ case have been discussed in Refs. [185, 186].

5.5 Conclusion:

We have shown how the Lippman-Schwinger formalism can be used to obtain exact results for two particles scattering from an interacting region. This method can also be applied to other cases, such as the two-wire system studied in Refs. [187, 188] or the case of spin-$1/2$ electrons as mentioned above. We have also demonstrated how the results of the scattering theory can be used to understand numerical results for a two-particle wave packet moving through the interacting region. Finally, we have considered the problem of many-particle transport across the interacting region; we find that the zero-temperature Landauer conductance is reduced by a term of order U^2. This calculation is nontrivial since it uses perturbation theory on many-particle scattering states and so is a fully nonequilibrium treatment. Many of the results presented here on scattering and bound states can be generalized to the case where the interaction occurs on more than one bond. Interestingly, in the presence of on-site eneries in the dot sites, first order change in the current due to interaction is order of U. So it is possible then to increase or decrease the current by tuning the interaction.

We would like to remark here that in a system in which the interacting region is much longer than k_F^{-1} and is connected adiabatically to leads where there are no interactions, it is known that the conductance remains equal to e^2/h; this is because momentum is conserved in such a system [193–197]. In our model, the interaction occurs only on one bond; thus the interaction changes rather abruptly in space. Hence momentum is not conserved (this is clear from the expression for the scattered state given in Eq. (5.6)), and the conductance is reduced from e^2/h.

A Heat transport in harmonic lattices

A.1 Green's function properties

We will consider some properties of the Phonon Green's functions. We denote by $\mathcal{G}^+(t)$ the full Green's function of the coupled system of wire and reservoirs. Let U and Ω^2 respectively denote the normal mode eigenvector and eigenvalue matrices satisfying the equations:

$$U^T \Phi U = \Omega^2, \quad U^T M U = \hat{I} \ . \tag{A.1}$$

We define the Green's function $\mathcal{G}^+(t)$ as

$$\mathcal{G}^+(t) = U \ \frac{\sin(\Omega t)}{\Omega} \ U^T \ \theta(t) \ . \tag{A.2}$$

It satisfies the equation

$$M\ddot{\mathcal{G}}^+(t) + \Phi \ \mathcal{G}^+(t) = \delta(t) \ \hat{I} \ . \tag{A.3}$$

The Fourier transform $\mathcal{G}^+(\omega) = \int_{-\infty}^{\infty} dt \ \mathcal{G}^+(t) e^{i\omega t}$ is thus given by

$$\mathcal{G}^+(\omega) = \frac{1}{-(\omega + i\epsilon)^2 M + \Phi} \ . \tag{A.4}$$

The isolated reservoir Green's functions are given by:

$$\begin{aligned} g_L^+(\omega) &= \frac{1}{-(\omega + i\epsilon)^2 M_L + \Phi_L} \\ g_R^+(\omega) &= \frac{1}{-(\omega + i\epsilon)^2 M_R + \Phi_R} \ . \end{aligned}$$

We can also represent $\mathcal{G}^+(\omega)$ as follows:

$$\begin{aligned} \mathcal{G}_{rs}^+(\omega) &= -\sum_Q \frac{U_{rQ} U_{sQ}}{(\omega + \omega_Q + i\epsilon)(\omega - \omega_Q + i\epsilon)} \\ &= -\sum_Q \frac{U_{rQ} U_{sQ}}{\omega^2 - \omega_Q^2} + \frac{i\pi}{2\omega} \sum_Q U_{rQ} U_{sQ} [\delta(\omega - \omega_Q) + \delta(\omega + \omega_Q)] \ . \end{aligned} \tag{A.5}$$

We will now express the wire-part of the full Green's function in terms of the uncoupled reservoir Green's functions. We write the equation for $\mathcal{G}^+(\omega)$ in the following form:

$$\begin{pmatrix} -M_W\ (\omega+i\epsilon)^2\hat{I}+\Phi_W & V_L & V_R \\ V_L^T & -M_L\ (\omega+i\epsilon)^2\hat{I}+\Phi_L & 0 \\ V_R^T & 0 & -M_R\ (\omega+i\epsilon)^2\hat{I}+\Phi_R \end{pmatrix} \times \begin{pmatrix} G_W^+ & G_{WL}^+ & G_{WR}^+ \\ G_{LW}^+ & G_L^+ & G_{LR}^+ \\ G_{RW}^+ & G_{RL}^+ & G_R^+ \end{pmatrix} = \begin{pmatrix} \hat{I} & 0 & 0 \\ 0 & \hat{I} & 0 \\ 0 & 0 & \hat{I} \end{pmatrix} . \tag{A.6}$$

From these equations we obtain the following expression for $G_W^+(\omega)$:

$$\begin{aligned} G_W^+(\omega) &= \frac{1}{-(\omega+i\epsilon)^2\ M_W+\Phi_W-\Sigma_L^+-\Sigma_R^+} , \\ \text{where}\quad \Sigma_L^+(\omega) &= V_L\ g_L^+(\omega)\ \ V_L^T\ , \\ \Sigma_R^+(\omega) &= V_R\ g_R^+(\omega)\ V_R^T\ . \end{aligned} \tag{A.7}$$

A.2 Equilibrium properties

In this section we will calculate the canonical ensemble expectation value of $K = \langle\ \dot{X}_W\dot{X}_W^T\ \rangle$ where the average is taken over the equilibrium density matrix of the entire coupled system of wire and reservoirs. Denoting by Z_Q the normal mode coordinates of the entire system we get, for points i, j on the wire:

$$\begin{aligned} K_{ij}^{eq} &= \langle \dot{X}_i\dot{X}_j\rangle_{eq} \\ &= \sum_Q U_{iQ}U_{jQ}\langle\dot{Z}_Q^2\rangle_{eq} \\ &= \sum_Q U_{iQ}U_{jQ}[\frac{\hbar\omega_Q}{2}+\hbar\omega_Q f(\omega_Q,T)] \\ &= \int_{-\infty}^{\infty} d\omega\frac{\omega}{\pi}\sum_Q U_{iQ}U_{jQ}\frac{\pi}{2\omega}[\delta(\omega-\omega_Q)+\delta(\omega+\omega_Q)]\frac{\hbar\omega}{2}\coth(\frac{\hbar\omega}{2k_BT}) \\ &= \int_{-\infty}^{\infty} d\omega\frac{\omega}{2\pi i}[(G_W^+-G_W^-)]_{ij}\frac{\hbar\omega}{2}\coth(\frac{\hbar\omega}{2k_BT}) . \end{aligned} \tag{A.8}$$

Now from Eq. (A.7) we have:

$$\begin{aligned} (G_W^-)^{-1}-(G_W^+)^{-1} &= (\Sigma_L^+-\Sigma_L^-)+(\Sigma_R^+-\Sigma_R^-)+4i\epsilon\omega M_W \\ &= 2\ i\ (\Gamma_L+\Gamma_R)+4i\epsilon\omega M_W \\ \Rightarrow G_W^+-G_W^- &= 2\ i\ G_W^+\ (\Gamma_L+\Gamma_R)\ G_W^-+4i\epsilon\omega\ G_W^+M_WG_W^- . \end{aligned} \tag{A.9}$$

Hence we finally get:

$$K_{ij}^{eq} = \int_{-\infty}^{\infty} d\omega \, \frac{\omega}{\pi} \, [\, G_W^+ \, (\Gamma_L + \Gamma_R) \, G_W^- \,]_{ij} \, \frac{\hbar\omega}{2} \, \coth(\frac{\hbar\omega}{2k_BT}) + \int_{-\infty}^{\infty} d\omega \, \frac{2\epsilon\omega}{\pi} \, [\, G_W^+ \, M_W \, G_W^- \,]_{ij} \, \frac{\hbar\omega}{2} \, \coth(\frac{\hbar\omega}{2k_BT}) \, . \tag{A.10}$$

Since we eventually take the limit $\epsilon \to 0$, the second term is non-vanishing only when the equation

$$Det[-\omega^2 M_W + \Phi_W - \Sigma_L^+(\omega) - \Sigma_R^+(\omega)] = 0 \tag{A.11}$$

has solutions for real ω. These solutions correspond to the *bound states*[2] of the coupled system of wire and reservoirs [32].

B Phenomenological decoherence and dissipation

B.1 Evaluation of Green's function for ordered chain

To find the Green's function we use the relation $G^{+}_{lm} = (\hbar/\gamma)Z^{-1}_{lm}$ where Z is a tridiagonal matrix with off-diagonal terms all equal to one. The diagonal terms are given by:

$$\begin{aligned} Z_{11} = Z^{+}_{NN} &= A(\omega) = \frac{\hbar}{\gamma}\left[\omega - \frac{\gamma^2}{\hbar^2} g^{+}(\omega)\right] \\ Z_{ll} &= B(\omega) = \frac{\hbar}{\gamma}\left[\omega - \frac{\gamma'^2}{\hbar^2} g^{+}(\omega)\right] \quad \text{for} \quad l = 2, 3 \ldots N-1 \ . \end{aligned} \tag{B.1}$$

The function $g^{+}(\omega)$ can be obtained from the green function of an isolated semi-infinite one-dimensional chain and, in the region of interest here ($|\hbar\omega| < 2\gamma$) is given by

$$g^{+}(\omega) = \frac{\hbar}{\gamma}\left[\frac{\hbar\omega}{2\gamma} - i\left(1 - \frac{\hbar^2\omega^2}{4\gamma^2}\right)^{1/2}\right] \ . \tag{B.2}$$

Using standard matrix manipulations we can evaluate the inverse of Z and find

$$\begin{aligned} Z^{-1}_{lm} &= (-1)^{l+m}\frac{D_{l-1}D_{N-m}}{\Delta_N} \quad \text{for} \quad m > l \\ &= (-1)^{l+m}\frac{D_{m-1}D_{N-l}}{\Delta_N} \quad \text{for} \quad m \le l \\ \text{where} \quad D_l &= AY_{l-1} - Y_{l-2} \\ \Delta_N &= Det[Z] = A^2Y_{N-2} - 2AY_{N-3} + Y_{N-4} \\ Y_l &= \frac{\sinh[(l+1)\alpha]}{\sinh(\alpha)} \\ \text{with} \quad e^{\pm\alpha} &= \frac{B}{2} \pm (\frac{B^2}{4} - 1)^{1/2} \ . \end{aligned} \tag{B.3}$$

We will assume that the root α has been chosen such that $\alpha_R = Re[\alpha] > 0$. Using the above results for the inverse of the matrix Z we find that for large N the Green's function in the wire is given by:

$$G^{+}_{lm} = \frac{(-1)^{l+m}\hbar}{2\gamma\sinh\alpha}\left[e^{-|l-m|\alpha} - \frac{(A - e^{\alpha})}{(A - e^{-\alpha})}\left(e^{-(l+m-2)\alpha} + e^{-(2N-l-m)\alpha}\right)\right] \tag{B.4}$$

B.2 Green's functions for the open ring

The full Green's function is given as $G^{+}_{lm} = (\hbar/\gamma)Z^{-1}_{lm}$ where Z is a near circulant matrix with off-diagonal terms $Z_{N1} = Z_{l\ l+1} = e^{-i\theta}$ for $l = 1, 2...N-1$ and $Z_{1N} = Z_{l-1\ l} = e^{i\theta}$ for $l = 2, 3...N$. The diagonal terms are given by:

$$\begin{aligned} Z_{11} &= Z^{+}_{MM} = A(\omega) = \frac{\hbar}{\gamma}\left[\omega - \frac{\gamma''^2}{\hbar^2}g^{+}(\omega)\right] \quad \text{with} \quad \gamma'_1 = \gamma'_M = \gamma'' \ , \\ Z_{ll} &= B(\omega) = \frac{\hbar}{\gamma}\left[\omega - \frac{\gamma'^2}{\hbar^2}g^{+}(\omega)\right] \quad \text{for} \quad l = 2, 3...M-1, M+1...N \ . \end{aligned} \tag{B.5}$$

Now using the method of Ref. [65] to determine inverse and determinant of the tri-diagonal matrix, we can find required inverse and determinant of the near circulant matrix Z through simple but tedious algebra.

$$\begin{aligned} \Delta_N &= \left((A - 2\cosh\alpha)^2(\cosh[N\alpha] - \cosh[p\alpha]) - 4\sinh^2\alpha((-1)^N\cos[N\theta] - \cosh[N\alpha])\right. \\ &+ \left. 4\sinh\alpha\sinh[N\alpha](A - 2\cosh\alpha)\right)/(2\sinh^2\alpha) \quad \text{with} \quad e^{\pm\alpha} = \frac{B}{2} \pm (\frac{B^2}{4} - 1)^{1/2} \end{aligned} \tag{B.6}$$

with $p = N_2 - N_1$. Similarly, the co-factor can be evaluated following the above trick. Here we find first C_{1M} and calculate $|C_{1M}|^2$ which is relevant to determine conductance $G(\phi)$ of the asymmetric ring between the drain and source contacts.

$$\begin{aligned} |C_{1M}|^2 &= 2\left[\cosh N\alpha_R\cosh p\alpha_R - \cos N\alpha_I\cos p\alpha_I + (-1)^N\{\cos N\theta\ (\cos p\alpha_I\cosh N\alpha_R - \cos N\alpha_I\right. \\ &\left. \cosh p\alpha_R) + \sin N\theta\ (\sin p\alpha_I\sinh N\alpha_R - \sin N\alpha_I\sinh p\alpha_R)\}\right]/(\cosh 2\alpha_R - \cos 2\alpha_I) \end{aligned} \tag{B.7}$$

where α_R and α_I are respectively real and imaginary part of α. For $\gamma' = 0$, the real part of α vanishes and the coefficient of $\sin N\theta$ in $|C_{1M}|^2$ also disappears. We denote, $|C_{1M}|^2_{\gamma'=0}$ by $|C^0_{1M}|^2$ and $|\Delta_N|_{\gamma'=0}$ by $|\Delta^0_N|$.

Finally we evaluate the Green's function of Eq. (3.41), where a single Büttiker probe is coupled to a middle site (l) of the open ring. Here again $Z_{11} = Z^{+}_{MM} = A(\omega)$, but all other diagonal terms are $\hbar\omega/\gamma$ except $Z_{ll} = B(\omega)$. The off-diagonal terms remain the same as before. Following the above method we calculate the Green's function ($l < M$)

$$\begin{aligned} G^{+}_{l1} &= \frac{(-1)^{l+1}\hbar}{2\gamma\Delta'_N\sinh^2\alpha'}\left[e^{i(l-1)\theta}\{B(\cosh[(N-l+1)\alpha'] - \cosh[(r+1)\alpha']) - 2\cosh[(N-l)\alpha']\right. \\ &\left. + \cosh[r\alpha'] + \cosh[(r+2)\alpha']\} + (-1)^N e^{i(l-N-1)\theta}(\cosh[l\alpha'] - \cosh[(l-2)\alpha'])\right] \\ &\text{with} \quad e^{\pm\alpha'} = \frac{\hbar\omega}{2\gamma} \pm (\frac{\hbar^2\omega^2}{16\gamma^2} - 1)^{1/2} \ , \end{aligned} \tag{B.8}$$

where $r = N - 2M + l$. In this case, we do not require to determine Δ'_N, the determinant of Z, as it gets cancelled in Eq. (3.41). Similarly G^{+}_{lM} can be evaluated.

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