Dirty Hubbard rings: renormalization group and exact diagonalization studies

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We studied mesoscopic Hubbard rings with impurities using the renormalization group (RG) technique and the exact diagonalizations. The exact diagonalization calculations showed that the charge stiffness normalized by the value of clean system has a peak as a function of electron-electron interactions. Previous RG analysis has succeeded to show the enhancement of the stiffness at weak interactions, but does not show the peak behavior. We derived RG equations with 4$k_F$ impurity scattering term, which was ignored in the previous studies, and reproduced the overall behavior of the exact diagonalization results.

I. INTRODUCTION

Low dimensional systems often show interesting quantum phenomena, and there particle-particle interactions and impurities sometimes play crucial roles. Mesoscopic rings are known to be one of the good examples and have been studied over the last few years in particular. When an external flux is applied through a mesoscopic ring, the current flows along the ring and the magnitude and the direction of the current changes as a function of the applied flux. The current flows in equilibrium and is therefore called persistent current. The presence of persistent current was first predicted by Byers and Yang, and Büttiker et al. [1], and observed in several recent experiments [2]. The magnitude of the observed persistent current is, however, much larger than the theoretical value calculated for non-interacting electrons with impurities [3], and therefore we need to take account of other factors. The factors, other than impurities, that might affect the persistent current are, for example, particle-particle interaction, periodic potential, spin degree of freedom, and multichannels. If the system has only one of these, the situation is rather simple and we believe we already well understand it. Impurities would reduce the persistent current [3]. Interactions would not change the persistent current [4]. Periodic potentials would change the shape of the persistent current as a function of the applied flux, but would not change its magnitude very much [6]. Spin degree of freedom or multichannels just give some numerical factor to the magnitude of the persistent current.

Now let us consider the system that has two or more of the above factors. The role of each factor could be different in this case. In the presence of particle-particle interactions and impurities, for example, the persistent current decreases as the interactions increase [4], while the interaction is an irrelevant parameter when it exists with no other factors. In general [1], interaction becomes relevant if it coexists with translationally noninvariant factors. As this example shows, the situations when two or more factors coexist are usually complicated and therefore interesting. In this paper we focus on the system with impurities, interactions, periodic potentials, and spins. The most typical and maybe the simplest model that contains all of them would be dirty Hubbard ring. Dirty Hubbard ring has been recently studied analytically [7,8] and numerically [10,11]. Giamarchi and Shastry [7] showed using the renormalization group (RG) analysis that repulsive interactions between particles would enhance the persistent current while they would suppress the persistent current in spinless fermion systems [12,13]. The persistent current does not continue to be enhanced, however, as we increase the interactions further. The exact diagonalization calculations [10,11] show that the persistent current has a peak at a characteristic interaction strength and begins to be suppressed by the interaction beyond that point. Two origins are expected to give the suppression. One is periodic potential. Even in the absence of impurities, interactions would suppress the persistent current on a lattice and the suppression is more emphasized as the particle density approaches to the half filling. This effect would exist in the dirty systems. The second origin that would suppress the persistent current would be the 4$k_F$ Fourier component of impurity scatterings. For strong electron-electron interactions, Hubbard model approaches to a spinless fermion model, and the 4$k_F$ scatterings in Hubbard model corresponds to the 2$k_F$ scatterings in the spinless fermion model. Since it is known [12,13] that the 2$k_F$ scatterings in the spinless fermion model would suppress the persistent current, we expect the 4$k_F$ scatterings would also suppress the persistent current of Hubbard model. The previous RG equations do not contain the 4$k_F$ scattering term and are not complete to reproduce the numerical results. We will derive RG equations taking account of the 4$k_F$ scatterings and will show the peak behavior of the persistent current.

The paper is organized as follows. In Sec. 2 we show the results of our exact diagonalization calculations. RG analysis is given in Sec. 3. Section 4 is devoted to summary of this study.
II. NUMERICAL RESULTS

We first show our exact diagonalization results, which are basically the same calculations as the previous ones \cite{10,11}. We used the modified Lanczos method \cite{15} to calculate the ground state energy \( E \) of Hubbard ring:

\[
H = -t \sum_{<ij>,\sigma} e^{i2\pi \phi_i/\phi_0} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i\sigma} V_{\text{imp}}(i) n_{i\sigma}
\]  

(1)

as a function of the applied flux \( \phi \). We assumed the uniform probability for the impurity potential \( V_{\text{imp}} \) between \(-W \) and \( W \). The impurity average of the energy \( E \) was taken over 512 to 3072 realizations. The persistent current \( I(\phi) \) is given by the first derivative of the averaged energy with respect to the flux \( \phi \), and the charge stiffness \( D_c \) is proportional to the second derivative of the energy. Since it is easier to calculate the charge stiffness than to calculate the persistent current in the RG analysis, and since the charge stiffness is a measure of the persistent current \cite{7,14}, we here show the results of the charge stiffness calculations. In the calculations we always chose even number of particles per spin. The reason is the following. For simplicity, let us consider free electrons with the numbers of up and down spins, \( N_\uparrow \) and \( N_\downarrow \), being equal. The ground state energy of the free electrons changes as we change the particle number per spin, \( N_\sigma \), from even to odd, and it has the relation \( E_{\text{even}}(\phi) = E_{\text{odd}}(\phi + \phi_0/2) \) where \( \phi_0 \) is the flux quanta. If we define the charge stiffness by \( D_c = (L/2) \partial^2 E(\phi)/\partial \phi^2 \big|_{\phi=0} \), the stiffness as a function of the particle density, does not change smoothly when \( N_\sigma \) moves between even and odd. We can avoid this problem if we take the second derivative at \( \phi = 0 \) when \( N_\sigma \) is odd, and at \( \phi = \phi_0/2 \) when \( N_\sigma \) is even. This causes another problem, however. In \( U \to \infty \) limit Hubbard model becomes the free spinless fermion model, where the particle number is always even since \( N_\uparrow = N_\downarrow \). Therefore we should take the derivative of the ground state energy at \( \phi = \phi_0/2 \) in \( U \to \infty \) limit although the derivative has to be taken at \( \phi = 0 \) at small \( U \). If we choose \( N_\sigma \) to be even, the system is always in the ‘even number’ sector in both limits of \( U = 0 \) and \( U \to \infty \), and we do not have to change the definition of the stiffness. For this reason, we chose even number of particles per spin and used the definition \( D_e = (L/2) \partial^2 E(\phi)/\partial \phi^2 \big|_{\phi=\phi_0/2} \) in the following exact diagonalization calculations.

Figure (1) shows the charge stiffness \( D_c \) as a function of \( U/t \) in the system of \( L=6 \) and \( N_\uparrow = N_\downarrow = 2 \). As observed in the previous exact diagonalization studies \cite{10,11}, it has a peak, and the peak position shifts towards higher \( U/t \) for the stronger impurity potential. The enhancement at small \( U \) is due to the impurity scatterings, since we know the charge stiffness in the clean systems, \( D_c(W = 0) \), decreases monotonically as \( U \) becomes larger. If we normalize the stiffness by \( D_e(W = 0) \), the peak still exists and the peak positions are located almost in the same place for the different impurity strengths (Fig. (2)). Since the normalization effectively eliminates the periodic potential contribution, Fig. (3) suggests that the reduction of the charge stiffness at large \( U \) is not only due to the periodic potentials but also due to the impurities. In the next section we will try to reproduce this behavior of the charge stiffness using the RG technique.

III. RG CALCULATIONS

One dimensional Hubbard model with impurities can be written in the boson representation by the following Lagrangian:

\[
L = L_\rho + L_\sigma + L_g + L_{2k_F} + L_{4k_F},
\]  

(2)

where

\[
L_\nu = \frac{1}{2\pi K_\nu} \int dx \{ u_\nu^{-1} (\partial_{x} \phi_\nu(x, \tau))^2 + u_\nu (\partial_{\tau} \phi_\nu(x, \tau))^2 \},
\]

\[
L_g = \frac{2g_{1,\perp}}{(2\pi \alpha)^2} \int dx \cos(\sqrt{2} \phi_\sigma(x, \tau)),
\]

\[
L_{2k_F} = \frac{1}{\pi \alpha} \int dx \xi_2(x) e^{i\sqrt{2} \phi_\sigma(x, \tau) + 2k_F x} \cos(\sqrt{2} \phi_\sigma(x, \tau)) + h.c,
\]

\[
L_{4k_F} = \frac{1}{\pi \alpha} \int dx \xi_4(x) e^{i\sqrt{2} \phi_\sigma(x, \tau) + 4k_F x} + h.c,
\]

\( \nu = \rho, \sigma \), and \( \alpha \) is the lattice constant. The last two terms in Eq. (2) represent the \( 2k_F \) and \( 4k_F \) Fourier components of impurity scatterings, respectively. The parameter \( g_{1,\perp} \) is equal to \( U \alpha \), where \( U \) is the on-site repulsion of Hubbard model. We assume gaussian distribution for the random fields \( \xi_2 \) and \( \xi_4 \): \( P(\xi_2) = N_2 \exp(-\int |\xi_2(x)|^2 dx/W_2) \) and
\[ P(\xi_4) = N_4 \exp(-\int |\xi_4(x)|^2 dx/W_4), \]
where \( N_2 \) and \( N_4 \) are the normalization factors. We did not include the forward scattering due to impurities because it can be eliminated by redefining the field \( \phi_\rho \)[3].

With help of the replica trick, we can integrate out the random fields \( \xi_4 \) and the final form of the action is

\[ S = S_\rho + S_\sigma + S_g + S_2k_F + S_4k_F, \]

where

\[ S_\nu = \sum_{i} \frac{1}{2\pi K_\nu} \int dx d\tau \{ u_\nu^{-1} (\partial_\nu \phi_\nu^i(x, \tau))^2 + u_\nu (\partial_x \phi_\nu^i(x, \tau))^2 \}, \]

\[ S_g = \sum_{ij} \frac{2g_{1\bot}}{(2\pi \alpha)^2} \int dx d\tau \cos(\sqrt{8} \phi_\nu^i(x, \tau)), \]

\[ S_{2k_F} = \sum_{ij} \frac{W_2}{(\pi \alpha)^2} \int dx d\tau d\tau' \cos(\sqrt{2} \phi_\nu^i(x, \tau)) \cos(\sqrt{2} \phi_\nu^j(x, \tau')) \cos(\sqrt{2}(\phi_\rho^i(x, \tau) - \phi_\rho^j(x, \tau'))), \]

\[ S_{4k_F} = \sum_{ij} \frac{W_4}{(\pi \alpha)^2} \int dx d\tau d\tau' \cos(\sqrt{8}(\phi_\nu^i(x, \tau) - \phi_\rho^j(x, \tau'))). \]

where \( i \) and \( j \) are the replica indices. Now we are ready to derive the RG equations. Up to the lowest order of \( g_{1\bot}, W_2 \) and \( W_4 \), the RG equations are obtained in the following form:

\[ \frac{dK_\rho(l)}{dl} = -\frac{1}{2} \left( \frac{K_\rho^2 u_\rho}{u_\sigma} \right) (\Delta_2(l) + \Delta_4(l)), \]

\[ \frac{du_\rho(l)}{dl} = -\frac{1}{2} \left( \frac{K_\rho u_\rho^2}{u_\sigma} \right) (\Delta_2(l) + \Delta_4(l)), \]

\[ \frac{dK_\sigma(l)}{dl} = -\frac{1}{2} K_\rho^2 (\Delta_2(l) + y(l)^2), \]

\[ \frac{du_\sigma(l)}{dl} = -\frac{1}{2} K_\sigma u_\sigma \Delta_2(l), \]

\[ \frac{dy(l)}{dl} = (2 - 2K_\sigma(l)) y(l) - W_2(l), \]

\[ \frac{\Delta_2(l)}{dl} = (3 - K_\rho(l) - K_\sigma(l) - y(l)) \Delta_2(l), \]

\[ \frac{\Delta_4(l)}{dl} = (3 - 4K_\rho(l)) \Delta_4(l), \]

where \( y = g_{1\bot}/\pi u_\sigma \), \( \Delta_2 = (2W_2/\pi u_\rho^2)(u_\sigma/u_\rho)K_\rho \), and \( \Delta_4 = 8W_4/\pi u_\sigma^2/\pi u_\rho^2 \). If we ignore the \( 4k_F \) scatterings, i.e. if we set \( W_4 = 0 \), the RG equations reduce to the ones derived by Giamarchi and Schulz [9].

We solved the Bethe ansatz equations of clean Hubbard ring [16,17] to determine the initial values for the integration of the RG equations. From the Bethe ansatz equations we obtain the stiffness and the susceptibility of charge and spin sectors. The parameters \( K \)'s and \( u \)'s can then be calculated from the following relations [17,3]:

\[ K_\rho = \frac{\pi u_\rho}{2} \sqrt{2D_\rho \chi_\rho}, \]

\[ u_\rho = \frac{2}{\rho} \sqrt{\frac{D_\rho}{2 \chi_\rho}}, \]

\[ K_\sigma = \pi \rho \sqrt{2D_\sigma \chi_\sigma}, \]

\[ u_\sigma = \frac{4}{\rho} \sqrt{\frac{D_\sigma}{2 \chi_\sigma}}, \]

where \( D_\nu \) and \( \chi_\nu \) are, respectively, the stiffness and the susceptibility of the \( \nu(= \rho, \sigma) \) sector and \( \rho \) is the particle number density. Note that the first two equations in Eq. [3] are exact, while the last two are approximate and valid when \( U/t \) is small [17,3].
Using the obtained parameters as the initial value of the RG equations, we integrated the equations numerically and stopped when $l$ reached $\log(L/\alpha)$. Figure 3 shows the normalized charge stiffness $D_c(W = 0)$ calculated with $W_4 = 0$. As obtained by Giamarchi and Shastry [7], the stiffness grows as the interactions increase, and never drops down. When $W_4$ is finite, however, the normalized charge stiffness has a peak as seen in Fig. 4. The peak stays almost in the same position for the different impurity potential strengths, and this feature is also observed in the exact diagonalization calculations. We therefore believe the RG equations (4) are complete to reproduce the qualitative feature of the exact diagonalization calculations.

IV. SUMMARY

The previous RG calculations that contain the $2k_F$ impurity scatterings succeeded to show the enhancement of the charge stiffness by the interaction $U$, which is an opposite feature to the spinless fermion systems where the interactions would suppress the stiffness. As we increase $U$ further, however, the exact diagonalization studies show the stiffness starts to decrease making a peak at a characteristic $U$. The peak behavior still exists even when we plot the normalized stiffness $D_c(W)/D_c(W = 0)$ as a function of $U$. This feature cannot be obtained from the previous RG equations and we need to take account of the missing term in their calculations.

We derived the RG equations for the dirty Hubbard rings with the $4k_F$ as well as the $2k_F$ impurity scatterings being included, and calculated the charge stiffness $D_c$ for various impurity strengths $W$ and electron-electron interactions $U$. At $U = \infty$ the Hubbard model is equivalent to the free spinless fermion model, where fermi wave vector is twice as large as the one of the original Hubbard model. Therefore the $4k_F$ scatterings become dominant as we approach $U/t \rightarrow \infty$ limit. Since the RG and the numerical calculations for the spinless fermions showed interactions would suppress the charge stiffness in dirty systems, we can expect that the RG equations with the $4k_F$ term should give the decreasing behavior of the charge stiffness with increasing $U/t$. We numerically integrated the RG equations and the normalized stiffness of the results makes a peak at a certain $U/t$, while it grows monotonically without the $4k_F$ term. It is also found that the peak position does not change very much for different impurity strengths. These results are consistent to the numerical analysis.

If we ignore the $4k_F$ term in the RG analysis, the persistent current becomes close to the impurity-free case at large $U$. In real systems, however, the $4k_F$ scatterings do exist and the persistent current cannot reach the impurity-free value. Therefore, one-dimensional Hubbard rings may not be sufficient to explain the large persistent current observed in the experiments [2], and we should take account of other factors such as multichannels.

Let us close this paper by commenting on the Coulomb interaction cases. Since arbitrary weak Coulomb interaction in one-dimensional electron systems makes the $4k_F$ density correlation dominant and drives the system to a Wigner crystal [8], the $4k_F$ component of impurity scatterings always plays central roles, and the persistent current and the charge stiffness would always be suppressed by the Coulomb interactions as a consequence. The exact diagonalization calculations [1] actually show that the Coulomb interactions would suppress the persistent current unless the impurity potentials are too strong [9].

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