

**Persistent currents in small, imperfect Hubbard rings**

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We have done a study with small, imperfect Hubbard rings with exact diagonalization. The results for few-electron rings show that the imperfection, whether localized or not, nearly always decreases, but can also *increase* the persistent current, depending on the character of the imperfection and the on-site interaction. The calculations are generally in agreement with more specialized studies. In most cases the electron spin plays an important role.

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**I. INTRODUCTION**

The regime of experimental studies in small semiconductor heterostructures has gone from mesoscopic to nanoscopic within a few years. Especially electron traps have been under intensive study because of the discrete nature of energy levels and the resulting analogy with real atoms. The trapping potential has varied between parabolic (quantum dot) (Ref. 1) and ringlike (quantum ring, QR).<sup>2-4</sup> While quantum dots fascinate because of the similarity with real atoms, rings combine this similarity with an always captivating ringlike geometry.

Rings are often studied with a relation to the persistent current (PC),<sup>5</sup> an equilibrium current that arises when an Aharonov-Bohm (AB) flux is piercing the ring.<sup>6</sup> Few-electron nanoscopic rings introduce many-body effects not observable in mesoscopic rings, such as the fractional  $\phi_0/N$  periodicity of the persistent current.<sup>7</sup> These systems have been studied theoretically, both in the single-particle<sup>8,9</sup> as well as in the many-body picture.<sup>10-13</sup> With continuum models, particularly in the analytical approach, it is laborious to introduce imperfections to a perfect ring, especially when nonperturbative treatment is required.

In addition to continuum models, lattice models have been applied to QR's.<sup>14-17</sup> If interactions are taken into account, the Hubbard model<sup>18</sup> is probably the most investigated model. Now, apart from being a toy model of mathematical physics,<sup>19</sup> the purpose of this paper is to show that a slightly generalized Hubbard model can also be an extremely valuable tool in getting the first idea of what is going on in small, numerically exactly diagonalizable systems. With the Hubbard model and exact diagonalization it is easy to introduce the effects, including an impurity, disorder, magnetic and electric fields, and external leads, which are much harder to include with other models. Here one does not need to limit to a certain region in the parameter space but can explore all the possible values of the parameters and we get an illustrative representation of the results.

The calculations show that imperfections mainly decrease the persistent current. The interaction, however, can introduce coupling of the two spin-currents and result in increase of the PC in certain situations, especially when the imperfection is of localizing nature. We conclude that spinless models cannot show these effects.

**II. THE MODEL**

We use the Hubbard Hamiltonian with a pure Aharonov-Bohm flux without a Zeeman term. In the presence of a vector potential the hopping integral is modified by a phase factor<sup>20</sup> and the Hamiltonian reads

$$H = - \sum_{i,j,\sigma} t_{ij} (e^{-ieA_{ij}/\hbar} c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{i,\sigma} \epsilon_i \hat{n}_{i\sigma}, \quad (1)$$

where we have generalized for site-dependent hopping integral as well as for one-body on-site energies  $\epsilon_i$ .  $A_{ij}$  represents the portion of the Aharonov-Bohm flux covered by the hopping  $i \leftrightarrow j$ , so that we could write the phase factor as  $\exp[-i(2\pi/L)(\phi/\phi_0)]$ , where  $L$  is the number of sites in the ring,  $\phi$  is the magnetic flux, and  $\phi_0 = h/e$  is the flux quantum. Energy scale is fixed by setting all  $t_{ij} = 1$  unless otherwise stated. Figure 1(a) shows examples of Hubbard rings considered in this research.

The dimension of  $H$  is

$$\binom{L}{N_\uparrow} \binom{L}{N_\downarrow},$$

where  $N_\sigma$  is the number of spin- $\sigma$  electrons, growing strongly with  $L$  and  $N_\sigma$ , limiting the system size. The diagonalization is done with standard library routines and the numerics do not involve severe difficulties.

The persistent current of an eigenstate  $\psi_m$  in a single ring is usually viewed via the expression  $I_m(\phi) = -\partial E_m / \partial \phi$ .<sup>21,22</sup> In the presence of multiple rings and different currents, however, we have to use the current operator. From the relation above and from the Feynman-Hellmann theorem we obtain<sup>23</sup>

$$\hat{j}_{kl\sigma} = \frac{4\pi t_{kl}}{\phi_0} \text{Im} [e^{-i(2\pi/L)(\phi/\phi_0)} c_{k\sigma}^\dagger c_{l\sigma}] \quad (2)$$

for the spin- $\sigma$ -electron current operator between the (irrelevant) sites  $k$  and  $l$ . The persistent current with the definition  $I(\phi) = -\partial E / \partial \phi$  is the sum of the two different spin currents. Using this operator is beneficial also because we obtain the current directly by taking the expectation value of operator (2) in a given state.

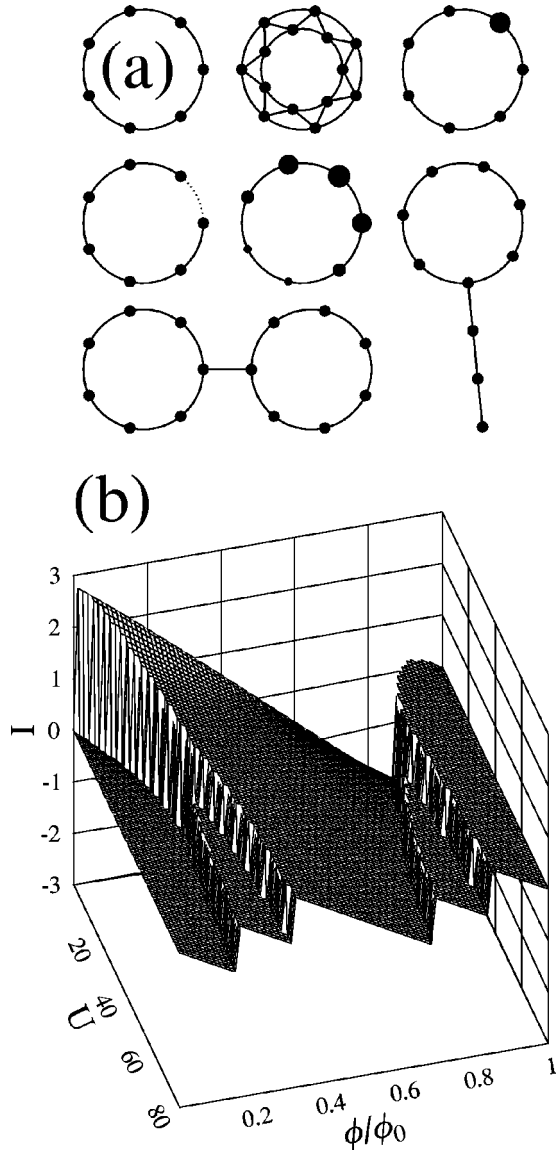


FIG. 1. (a) Structures of some of the Hubbard rings used in the calculations. The size of the point represents the on-site energy. The dashed line represents a weaker (or stronger) hopping probability. (b) Persistent current of a perfect ring with  $L=7$  and  $N_{\uparrow}=N_{\downarrow}=2$  as a function of the interaction  $U$  and the flux  $\phi$ . Note the periodicity change from  $\phi_0$  to  $\phi_0/N_e = \phi_0/4$  as the interaction increases.

The persistent current is a periodic function of  $\phi$  with periodicities  $\phi_0$ ,  $\phi_0/2$ , and  $\phi_0/N_e$  increasing with the interaction, as shown in Fig. 1(b). The periodicity has been studied before,<sup>7,24,25</sup> and the purpose of Fig. 1(b) is just to show that it makes sense to characterize the persistent current by fixing  $\phi$  as long as it does not contain any discontinuities. Like many other authors,<sup>12,14</sup> we have used the value  $\phi = 0.25\phi_0$  and the ground-state persistent current throughout the paper.

It is suggestive that in the Hubbard model the quasi-one-dimensionality can be mimicked by adjusting the interaction term: A Hubbard ring with multiple channels [Fig. 1(a)] and  $U \gg 1$  is mimicked by a single channel and a relatively small  $U$ .<sup>25</sup> Thus the Hubbard  $U$  in these ringlike structures can be

read either as an interaction as such or as a measure of the one-dimensionality of the ring.

### III. RESULTS AND DISCUSSION

The effect of a single impurity on PC has been studied by several authors.<sup>12,26,27,36</sup> Figure 2(a) shows PC influenced by an on-site energy  $\epsilon_1$  and the interaction. With zero impurity, the current decreases when the interaction  $U$  (or one-dimensionality) increases. This happens because with increasing  $U$  Hamiltonian (1) prevents electrons from moving independently and eventually only rotation as a rigid rotor is possible. These observations are in agreement with more specialized papers.<sup>12,28</sup>

The current always decreases monotonously with increasing positive  $\epsilon_1$ . Investigating Fig. 2(a) more carefully with a fixed positive impurity, one can see that there is a slight increase of the current with the interaction. This result, confirming earlier calculations,<sup>29-31</sup> tells that a greater interaction makes the electron system more correlated, pushing the impurity-affected electrons more effectively. Because there are observations contradicting this result,<sup>26</sup> saying that in the presence of impurity the interactions suppress PC even further, we hasten to add that with  $\epsilon_1 > 0$  the current with large enough interaction is slightly smaller than the current without interaction. Note that in the case of, for example, the Coulomb potential, the interaction is either on or off, and this kind of gradual increase in the interaction strength is usually not considered. However, as discussed above, the increase of electron-electron interaction corresponds to a decrease of the width of the quasi-one-dimensional ring.

With often disregarded attractive impurity and fixed  $U$  one can see a local maximum of  $I$  with specific  $\epsilon_1$ . Here the impurity localizes electrons, and if the depth of the impurity potential is equal to the interaction,  $U + \epsilon_1 = 0$ , the electrons with the opposite spin do not feel any extra on-site energy as an effect and thus pass the impurity unaffected. Either increasing or decreasing  $U$  (or  $\epsilon_1$ ) makes the effective on-site energy repulsive or attractive, on decreasing  $I$ . Away from this region of local maximum (especially with  $U=0$ ) the attractive impurity decreases the current more effectively than the repulsive one.

A similar effect is seen in Fig. 2(b), where the “impurity” is now a different hopping integral  $t_{12}$ . The current goes to zero with  $t_{12}$  as it should, but surprisingly, it has a maximum near  $t_{12} \sim 1$ , above which it decreases. The physics is the same as with attractive impurity, because the large negative kinetic energy of the strong link localizes an electron pair to the corresponding sites, creating a similar kind of blocking effect; note that the form of Fig. 2(b) with  $t_{12} > 1$  is the same as that in Fig. 2(a) with  $\epsilon_1 < 0$ .

Because we have an equal number of electrons with the opposite spin, the different spin currents, by symmetry, are the same. But if  $N_{\uparrow} \neq N_{\downarrow}$ , they are in the opposite direction. This can be seen in Figs. 2(c) and 2(d), which show spin-up and spin-down currents as a function of  $U$  and the single impurity strength for  $N_{\uparrow}=2$  and  $N_{\downarrow}=1$ . The opposite signs and relative magnitudes of PC with zero interaction and impurity, i.e.,  $I_{\uparrow}(0,0)/I_{\downarrow}(0,0)$ , can in fact be easily explained

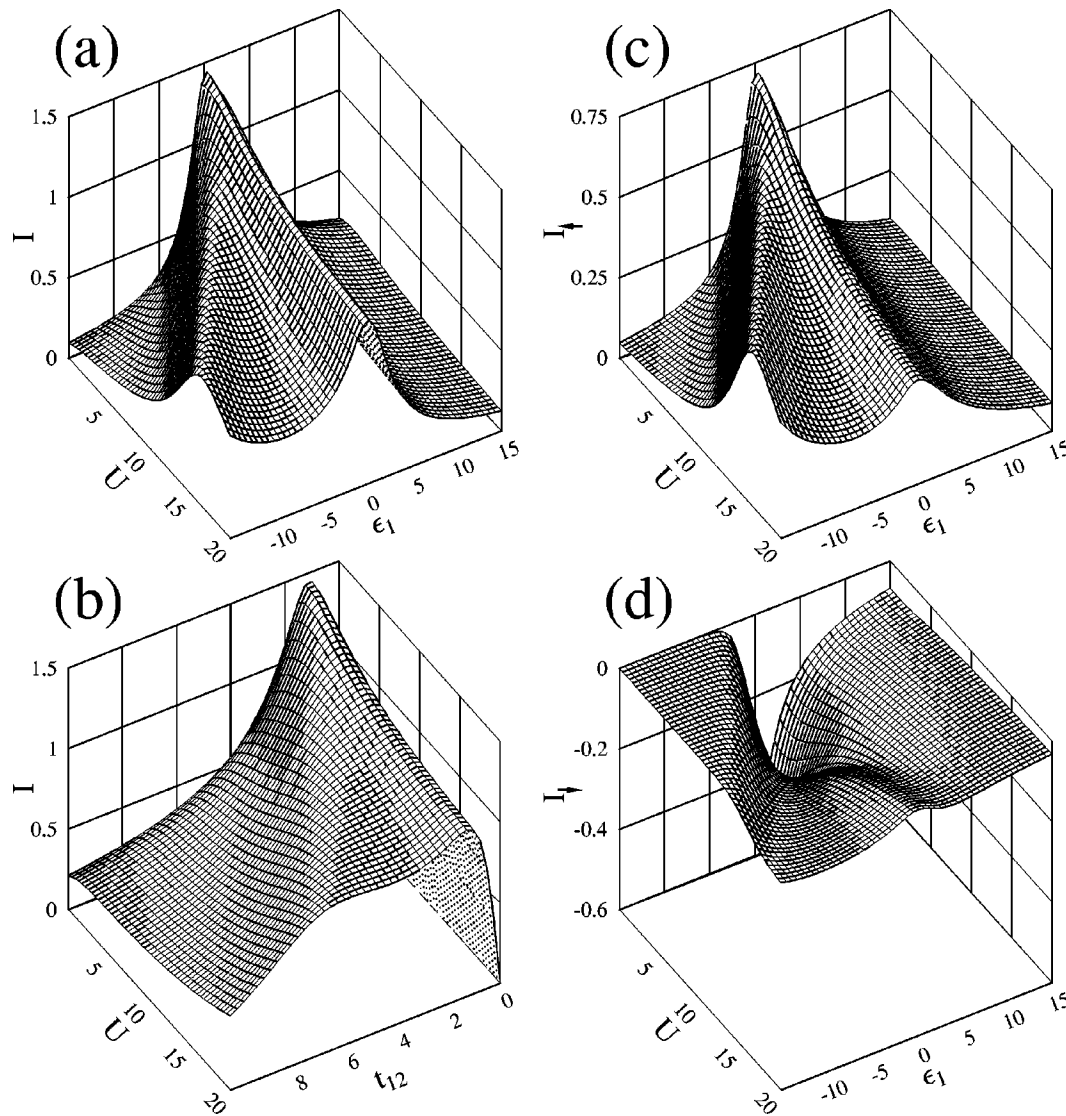


FIG. 2. Effect of a single impurity on the persistent current at a fixed value of flux ( $\phi=0.25\phi_0$ ). In (a) the impurity is described with an on-site energy  $\epsilon_1$ , in (b) with a hopping parameter  $t_{12}$  ( $L=7$ ,  $N_\uparrow=N_\downarrow=2$ ), and (c) and (d) show separately the spin-up and spin-down currents in the case of three electrons ( $L=7$ ,  $N_\uparrow=2$ ,  $N_\downarrow=1$ ) and a single impurity described with  $\epsilon_1$ .

also with *noninteracting* electrons in a continuous, strictly one-dimensional ring. The effect of interaction is to “grab” the spin-down electron to move to the same direction as the spin-up electrons, leading eventually to the rigid rotation of the whole electron system. However, to the total current ( $I_\uparrow+I_\downarrow$ ) the impurity has the same effect in the three-electron case as in the four-electron case. With other odd numbers of electrons the situation is similar to that of the three-electron case.

A random external potential at the ring is often called disorder and its effect on PC and the energy spectra is largely studied subject mainly due to the relevance in experimental samples.<sup>14–16</sup> Figure 3(a) shows an ensemble averaged  $I(U,W)$ , where  $W$  is the measure of the disorder, defined as  $W=\max(\{\epsilon_i\})-\min(\{\epsilon_i\})$  with  $\{\epsilon_i\}$  being random on-site energies (the ensemble consisted of 60 rings). The current decreases monotonously with  $W$ , but the role of the interactions is again not trivial, since a given disorder strength gives the

current a maximum with  $U\sim W$ . The increase of PC with  $U$  ( $\ll 1$ ) has been confirmed by other authors.<sup>29,30</sup> Physically the maximum can again be explained by the effective potential smoothing that originates from the disorder-localized electrons and their repulsive interaction towards the electrons of opposite spin. The impact of interactions can be different in spinless models<sup>16</sup> (where intersite interaction is required, e.g., a Coulomb-like interaction term<sup>14</sup>). But at this point we want to stress that if the spin currents, potentially even of opposite sign, are present, then the effect of interaction, by coupling the two currents as described above, is quite subtle and differs from the effect in spinless models.

By comparing carefully Figs. 3(a) and 3(b), the resemblance is obvious. Figure 3(b) shows the same plot as Fig. 3(a) but now with disorder strength  $W$  replaced by the strength  $V_E$  of an electric field parallel to the plane of the quantum ring. The physics remain the same: while the field “inclines” the ring so that some electrons tend to roll down



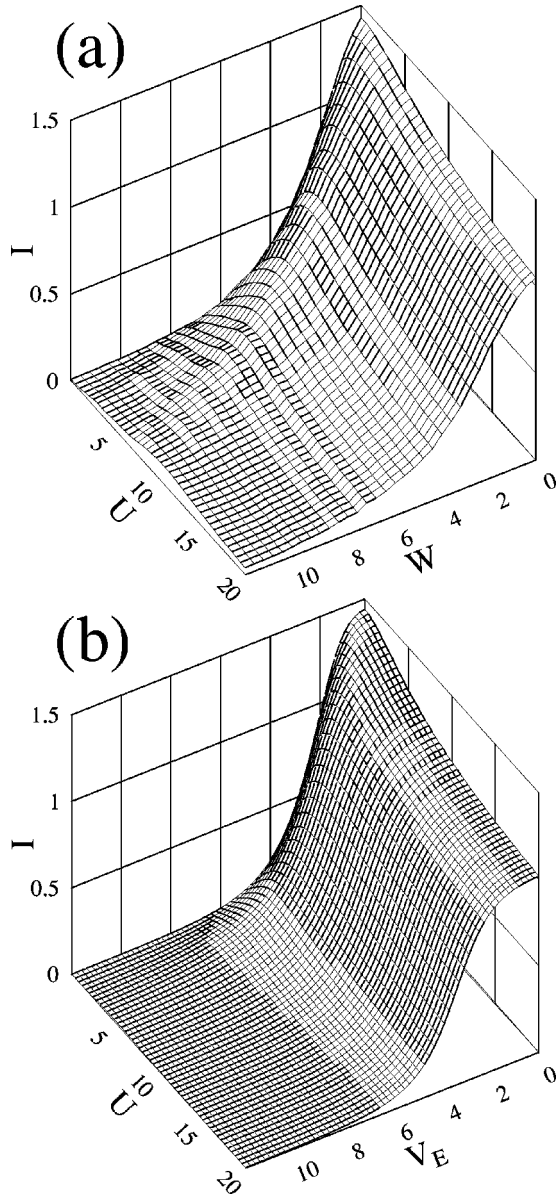


FIG. 3. Effect of random on-site energies (a) and electric field (b) on the persistent current at  $\phi = 0.25\phi_0$  ( $L = 7$ ,  $N_{\uparrow} = N_{\downarrow} = 2$ ).  $W$  is a measure of the disorder of the on-site energies and  $V_E$  is the strength of the electric field parallel to the plane of the ring.

to the other end of the ring, the interaction smoothens the way to the electrons of the opposite spin, creating an optimum interaction for given  $V_E$ . On the other hand, for a given  $U$  an increasing electric field destroys the Aharonov-Bohm oscillations, since the wave function does not extend throughout the whole ring.<sup>32</sup>

Finite temperature behavior of the persistent current is more intuitive, as seen in Fig. 4(a). The current decreases monotonously with  $U$  at all temperatures, and with a fixed  $U$  the current is almost constant for small enough  $T$ , until it decreases essentially to zero in the temperature range that is given by the energy gap between the ground state and the excited states. This is because the directions of the currents of the excited states are frequently opposite to the current of

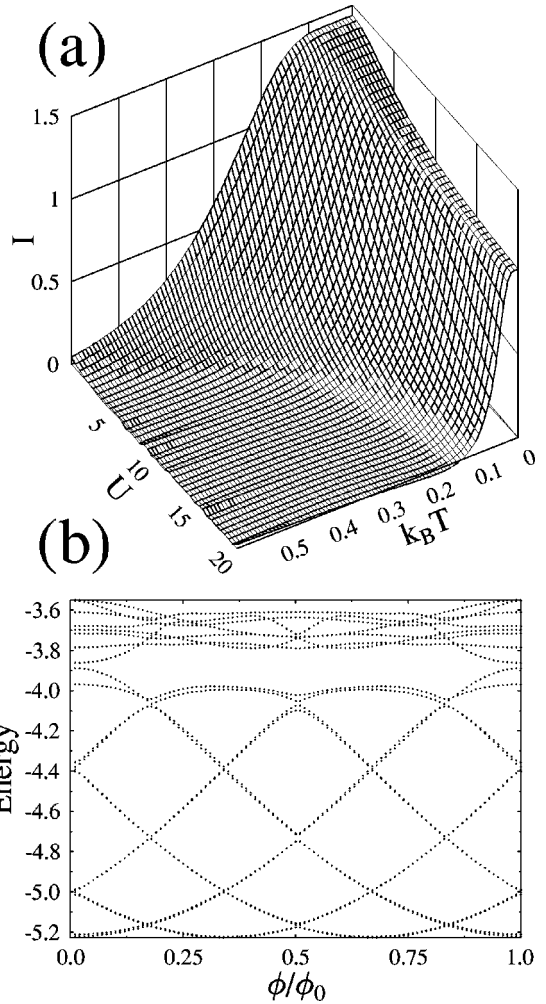


FIG. 4. (a) Temperature dependence of the persistent current in a perfect ring with  $L = 7$  and  $N_{\uparrow} = N_{\downarrow} = 2$  ( $k_B T$  measured in units of  $t$ ). (b) The energy spectrum  $E_i(\phi)$  of a ring with six sites and a stub with two sites [in 1(a) a related system is shown with a ring of seven sites and a stub of three sites]. The system has four electrons ( $N_{\uparrow} = N_{\downarrow} = 2$ ) and  $U = 1000$ . The low-energy spectrum is nearly identical with a spectrum of three electrons in a pure ring without the stub.

the ground state. The observations agree with the noninteracting picture of Refs. 15, 33.

As is the temperature, so are the external leads an inevitable imperfection in externally tuneable quantum rings.<sup>3,4</sup> With a lattice model one could imagine modeling these with an attractive on-site energy, larger hopping integral, or maybe with a smaller interaction term that is due to the larger space available in the vicinity of the leads. The ring-stub system, a schematic of which is shown in Fig. 1(a), has been studied by continuum models.<sup>34-37</sup> It was found that the stub can create standing waves that are not affected by the magnetic flux piercing the ring. With our approach, including now also the many-body effects, it is found that with large enough interaction, the stub of definite length can localize an integer number  $N_{stub}$  of electrons, and as a result the remaining electrons in the ring exhibit normal AB oscillations with  $N_e - N_{stub}$  electrons, as if the stub would be absent. This is

shown in Fig. 4(b), where we have a system of four electrons, but the low-energy spectrum is essentially the same as the pure-ring spectrum with just three electrons. If the stub length would be increased by one site, the standing wave would not have a node anymore at the stub-ring interface and the localized electron would start interfering with the electrons in the ring, suppressing the current.<sup>38,39</sup>

If the stub is connected to another quantum ring, as depicted in Fig. 1(a), we get coupled quantum rings, which could be experimentally realistic in a dense ensemble of self-assembled quantum rings.<sup>2</sup> Studied with noninteracting continuum electrons,<sup>40</sup> the relative directions of PC in coupled rings of different radii were found to depend on the magnetic flux. If we define a reference ring with length  $L_r$  to enclose a flux  $\phi_r$ , a ring with length  $L$  then encloses a flux  $\phi = (L/L_r)^2 \phi_r$ , and we can have rings of different sizes by applying the corresponding fluxes to the phase factor of the hopping integral in Hamiltonian (1). It is found that the currents in the rings of length  $L_1$  and  $L_2$  indeed run in the opposite direction if, e.g., the flux through the first ring is less and the flux through the second ring is more than integer multiple of a flux quantum.<sup>41</sup> Though we have two independent currents, it turns out that the derivative of the total energy resembles the sum of the currents very closely, and thus may lead to large periodicities if  $L_1/L_2$  differs only slightly from unity.

Most of the figures show results for rings with  $L=7$  and  $N_e=4$ , but it is important to point out that also other rings were investigated, giving similar results. We want to defend this choice by the notion that in the limit of large  $U$ , the Hubbard model becomes the Heisenberg model with an effective coupling constant  $J_{eff}$ ,<sup>17,25</sup> which, for large  $L$ , scales as  $J_{eff} \propto L^{-3}$ . This, together with our calculations, shows that the energy separations—and consequently the persistent current—decrease with  $L$ . This implies that the general trends depicted in the figures tend to diminish as the number

of empty lattice sites is increased. Furthermore, for these few-electrons systems, because of the *local* interaction, the model does not necessarily compare to real continuum models better if  $L$  is increased.

#### IV. CONCLUSIONS

To conclude, we have studied small imperfect Hubbard rings with exact diagonalization. The results show that the imperfection, whether localized or not, almost always decreases the persistent current. The interaction, however, can introduce coupling of the two spin-currents, making the effective potential felt by opposite-spin electrons smoother and result in increase of PC in certain situations, especially when the imperfection is of localizing nature. We note that these effects cannot be seen with spinless electrons. The decrease in PC as a function of impurity potential starts with zero slope. In pure rings the current decreases with temperature monotonously in a scale given by the energy gap above the ground state.

By comparing with other studies, it is shown that even these very small rings give the same physics and phenomena that is obtained with more involved Hubbard-model calculations, including, e.g., Bethe-Ansatz calculations. Furthermore, many realistic investigations with continuum models leave the phenomena obtained with this approach mainly intact.

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