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Persistent currents in disordered rings

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Numerical calculations are performed to determine how persistent currents in mesoscopic metallic rings are affected by a diagonal disorder. We use a tight–binding model with long–range hoppings and the hopping integrals are assumed in such a way, that the resulting electron dispersion relation is almost the same as for free electrons. We analyze one– and two–dimensional rings. We discuss the dependence of the amplitude of the persistent current on the concentration of impurities and on their potential.

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1. Introduction

There is a well–known problem connected with the amplitude of the persistent currents in mesoscopic rings. Namely, apart from ballistic regime, the magnitude of the measured current is two or three orders higher than predictions from one–electron theory.[1] On the other hand, currents measured in semiconductor rings with mean free path bigger than their circumference, remain in a good agreement with theory.[2] The last statement holds true even if the theoretical approach neglects the Coulomb interactions between electrons in the ring. It may suggest that the discrepancy that occurs for diffusive rings originates mainly from inadequate description of the influence of the disorder, rather than from the poor description of the electron-electron interactions. Still, there are many papers which demonstrate that this interaction can significantly enhance the current.[3] Therefore, it would be very useful to carry out calculations that account also for the Coulomb interaction. Unfortunately, it usually puts significant limits on the accessible size of the system under investigation (e.g. exact diagonalization[4]) or introduces hardly controllable, especially in low dimensional systems, approximations (e.g. mean-field type approaches). Therefore, in the present paper we focus on the role which disorder plays in small rings, being aware that our results can be modified when the Coulomb interactions are taken into account. We use a tight–binding Hamiltonian with long–range hopping and a diagonal disorder to describe one– and two–dimensional ring pierced by a magnetic flux. The hopping integrals are calculated from the condition that the resulting dispersion relation accurately fits that of the free electron gas. With the help of numerical diagonalization of the Hamiltonian we investigate how the persistent current depends on the disorder present in the ring.

The disorder in a ring can be characterized by the electron mean free path l. It is known that the typical current (root mean square current, $I_{\mathrm{typ}}=\langle I^2\rangle^{1/2}$) in a metallic ring is proportional to the mean free path l.[5] Depending on the realization of the disorder different formulas for l can be used and the comparison of the theoretical predictions with the numerical results can give us some information concerning the applicability of these formulas.

2. The model

The rings are described by the following tight–binding Hamiltonian

$$H=\sum_{i,j,\sigma} t_{ij}e^{iq_{ij}}c^{\dagger}_{i\sigma}c_{j\sigma}+\sum_{i\sigma} e_i n_{i\sigma}. \qquad (1)$$

Here, t_{ij} is the hopping integral between sites i and j, $c^{\dagger}_{i\sigma}$ creates an electron with spin σ at site i of the ring, $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$ and ε_i describes the disorder. The magnetic flux enters the Hamiltonian through the Peierls phase factor θ_{ij}, describing the orbital response of the system to an external magnetic field:

$$q_{ij}=\frac{2p}{F_0}\int_{\mathbf{R}_j}^{\mathbf{R}_i}\mathbf{A}\times d\mathbf{l}, \qquad (2)$$

where $\Phi_0=hc/e$ is the flux quantum.

Our aim is to describe electrons moving in a metallic ring, where, apart from scattering by impurities, in the vicinity of the Fermi level they behave like nearly free electrons. Therefore, the hopping integral t_{ij} is non-zero not only for nearest neighboring sites i and j. Instead, we allow for long–range hoppings, choosing the values of t_{ij} in such a way, that the resulting dispersion relation is close to that for free electrons. In the case of a two–dimensional ring the procedure consists in minimization of a function

$$f(t^{(1)},t^{(2)},t^{(3)},\ldots;k_x,k_y) - \sum_{k_x k_y}[E(t^{(1)},t^{(2)},t^{(3)},\ldots;k_x k_y) - (k_x^2+k_y^2)]^2 \qquad (3)$$

with respect to $\{t^{(n)}\}$. Here, $t^{(0)} \equiv t_{ii}$ is the atomic level in the absence of the disorder, $t^{(1)}$ stands for t_{ij} for nearest–neighboring (i,j), $t^{(2)}$ for next–nearest–neighboring (i,j), and so on, and $E(t^{(1)},t^{(2)},t^{(3)},\ldots;k_x,k_y)$ denotes the Fourier transform of t_{ij} for a given set of $t^{(n)}$'s. Relation (3) also defines the energy unit as $\hbar^2/2m$. In an analogous way the hopping integrals have been determined for one–dimensional rings.

It has been shown in Ref. [6] that in two– and three–dimensional rings the persistent current as a function of the magnetic flux strongly and irregularly depends on the number of electrons. This effect originates from numerous crossings between the energy levels. Each such a crossing leads to a jump in the flux dependence of the current. For a parabolic dispersion relation the low–laying states do not cross apart from $\Phi = n\Phi_0$ and these jumps do not occur in systems with low carrier concentration. Therefore, in order to avoid this drawback, we have restricted further analysis to systems with only two electrons with opposite spins. Since we neglect the many–body effects, this restriction does not strongly affect the results. This assumption has another advantage connected with this form of the dispersion relation. In a small ring its width limits the number of allowed hopping integrals $t^{(n)}$ and therefore fitting to parabolic dispersion relation is not possible over the whole Brillouin zone. Fortunately, if there are only few electrons in the ring, only shape of the bottom of the band matters. Therefore, the cosine functions occurring in the Fourier transformation of t_{ij} have been expanded around the point $(k_x,k_y)=(0,0)$ in two–dimensional case, and then fitted according to Eq. 3. It assures that at least at low temperature the lattice electrons will behave like free particles.

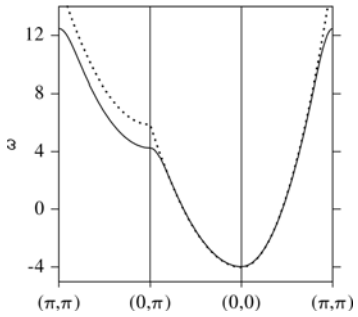

Fig. 1. Comparison of the dispersion relation for electrons described by a thigh–binding Hamiltonian with hoppings up to 18th nearest neighbors (solid line) with that of free electrons (dotted line).

Fig. 1 shows a comparison of two–dimensional dispersion relation obtained by taking into account all hoppings at range up to 18 lattice constants with a parabolic one and Figure 2 shows the difference between these two dispersion relations. The quality of the fit can also be seen in Figure 3, where the resulting density of states is compared to that of free electrons.

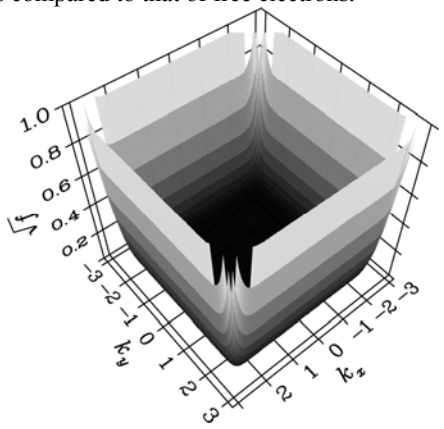

*Fig. 2. Deviation of the tight–binding dispersion relation from that for free electrons $\sqrt{f(k_x,k_y)}$ (Eq. **Error! Reference source not found.**) for momentum from the first Brillouin zone.*

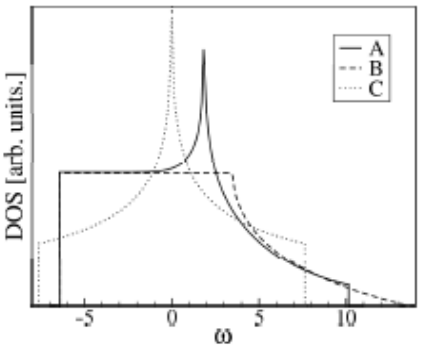

Fig. 3. Comparison of the density of states for electrons described by the hopping term with hoppings up to 18th nearest neighbors (A) fitted to free electron dispersion relation (B). The dotted line (C) shows the density of states for lattice electrons with only the nearest neighbor hoppings.

3. Numerical results

The typical current I_{typ} in a disordered ring depends on the actual realization of the disorder. In order to analyze this influence we have carried out simulations in two cases. First (case *A*), when there are some randomly chosen lattice sites (impurities) with atomic level shifted by a given energy with respect to the rest of the sites. We change both the concentration of the impurities as well as their potential (which is common to all of them). Such a system can be called a binary alloy.

In this case the electron mean free path within the Born approximation is[7]

$$l \propto \frac{1}{n_i U^2}, \tag{4}$$

where n_i is the concentration of impurities and U is the impurity potential, i.e., the atomic level of sites occupied by the impurities is given by $\varepsilon_{imp}=\varepsilon+U$, where ε is the common atomic level of the rest of the sites.

In the second case (case *B*, the Anderson model), the atomic levels of all sites are randomly chosen from a range of $(-W/2,W/2)$, where W determines the strength of the disorder. Since the persistent current strongly depends on the distribution of impurities or configuration of energy levels, for each set of parameters we have carried out numerous (up to one hundred) simulations, each time randomly generating disorder. Then the results were averaged over disorder realization. In this case elementary scattering theory says that the electron mean free path is[8]

$$l \mu \frac{1}{W^2}. \tag{5}$$

3.1 One–dimensional ring

In a one–dimensional ring consisting of N lattice sites we have taken into account all possible hoppings. Namely, using one–dimensional version of Eq. 3 we have determined $N/2$ hopping integrals. Figure 4 presents results for a disorder of type *A*: the lines show the typical current I_{typ} as a function of the concentration of impurities n_i. The current is averaged over 100 randomly generated configurations of the impurities. Different lines correspond to different values of the impurity potential U (upper panel) and to different impurity concentrations (lower panel). The inset in the lower panel shows a comparison of the results obtained for the model with hoppings up to 18th neighbor with results for the nearest neighbor hopping. Since the bandwidth is different in these cases, it is not obvious how to compare such results. It has been argued in Ref. [6] that taking into account long–range hopping integrals leads to an enhancement of the persistent current by an order of magnitude. However, the authors used the nearest neighbor hopping integral as the energy unit and all the long–range hopping integrals were positive. As a result in the case of long–range hoppings the bandwidth was much larger than for the nearest neighbor hopping and the ratio of the strength of the disorder to the bandwidth was much smaller. This can explain the enhancement of the persistent current. In order to avoid such a situation, in the case of only the nearest neighbor hopping we have assumed such a hopping integral which, in the absence of the disorder, gives the same value of the current as obtained for long–range hoppings. It can be easily shown that the assumption of the hopping integrals according to Ref. [6] leads to currents one or two orders of magnitude larger than within our approach. However, this enhancement occurs even in the absence of a disorder, i.e., for rings in the ballistic regime, where the magnitude of the observed current agrees reasonably well with a simple one–electron theory. Additionally, if the energy unit in the approach proposed in Ref. [6] is chosen in such a way that the typical current in the absence of the disorder is the same as in our approach, the dependence of the current on the strength of the disorder in both these approaches is almost the same.

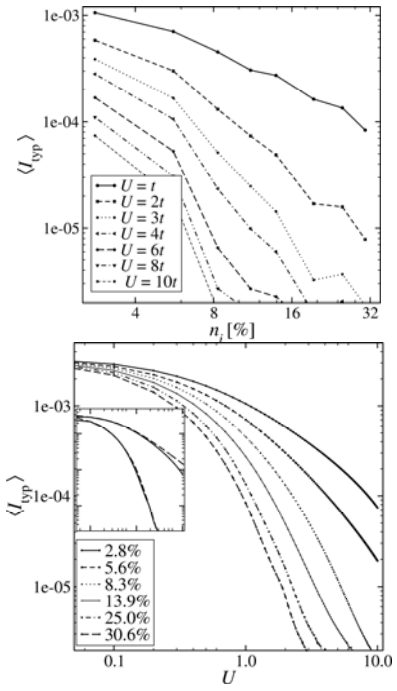

Fig. 4. Typical current averaged over 100 realizations of the disorder as a function of the impurity concentration (upper panel) and of the impurity potential (lower panel). Results obtained for a one–dimensional 36–site ring. The tails visible in the lower panel for high impurity concentrations are artifacts of the numerical procedures and originate from the long distance hoppings. They do not occur in the case of only the nearest neighbor hopping. The inset in the lower panel shows a comparison of the current for long–range hopping (solid lines) with results for the nearest neighbor hopping (dashed lines) for n_i equal to 2.8% and 30.6%. See text for details.

Fig. 4 presents data plotted in log-log scale. Therefore, if the simple approximation that leads to Eq. (4) was valid, and the system was in a diffusive regime, where $\langle I_{typ}\rangle \propto l$, the lines in both panels in Fig. 4 would be straight ones and parallel to themselves. Fig. 4 suggest that even for a medium values of U and n_i Eq. (4) cannot be applied to our system.

A slightly different situation occurs when the system is described by the Anderson model (case *B*). Figure 5 shows the typical current as a function of the disorder strength W. For W of the order of the bandwidth the results can be fitted by $\langle I_{typ}\rangle \propto W^{-x}$ but with x much larger than 2, what is in disagreement with Eq. (5). In fact, the section of

the curve which is straight in the log–log plot, can be fitted with $x \approx 4$, what indicates much faster suppression of the typical current by the disorder. Also in the case of the Anderson model, the correctly scaled results for only the nearest neighbor hopping (indicated in Figure 5 by the open circles) are almost indistinguishable from these for a long–range hopping.

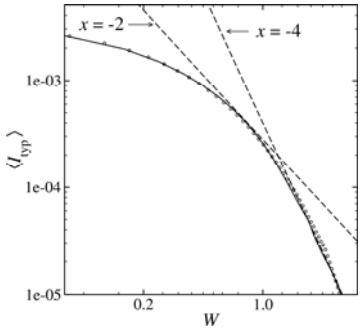

Fig. 5. Typical current averaged over 100 realizations of the disorder as a function of the disorder strength. Results obtained for a one–dimensional 36–site ring with site energies randomly chosen from a box distribution of width W. The solid line indicates results for long range hopping and the open circles for the nearest neighbor hopping. The dashed lines are of the form W^x.

3.2 Two–dimensional ring

Figs. 6 and 7 demonstrate the typical current as a function of the disorder strength. As expected, the reduction of the persistent current by disorder in the two dimensional case is less pronounced than for purely one dimensional rings. This can be inferred from the slopes of curves presented in Figs. 5 and 7. In the case *A*, the slope of curves plotted in the log–log scale strongly depends on the concentration of impurities what, similarly to the 1D, visibly differs from the bahavior expected on the basis of the Born approximation. As can be inferred from Fig. 6 long range hopping integrals do not influence the qualitative dependence of the persistent current on the impurity potential.

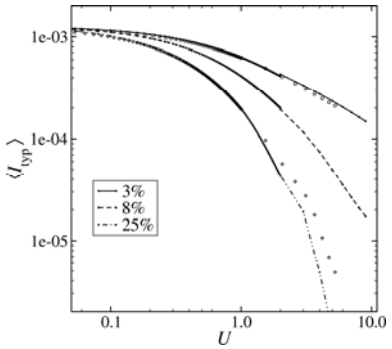

Fig. 6. The same as in Fig. 5, but for a 36×6 ring. The current has been averaged over 20 realizations of the disorder.

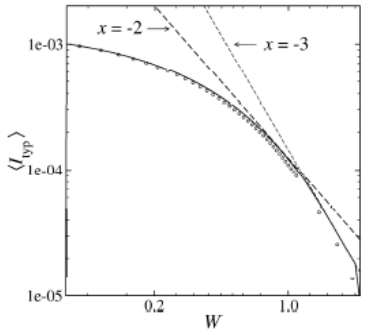

Fig. 7. The same as in Fig. 5, but for a 36×6 ring. The current has been averaged over 20 realizations of the disorder.

4. Concluding remarks

We have investigated the persistent current in a disordered one and two dimensional rings pierced by an external magnetic flux. Our aim was to find out whether the free electron dispersion relation suitable to describe metallic rings may suppress the reduction of the persistent current by disorder and explain the discrepancy between the experimental and theoretical results. Such a possibility has been suggested in Ref. [6], where the long range hopping has been included. Our results lead to an opposite conclusion. Although the long-range hopping integrals modify the magnitude of the persistent current, its dependence on the disorder remains almost the same as for the nearest neighbor hopping. This difference may originate from the choice of the hopping integrals. In Ref. [6] all the hopping integrals are positive, whereas our fitting procedure leads to positive as well as negative hopping integrals.

Acknowledgements

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References

[1] L. P. Lévy, G. Dolan, J. Dunsmuir, H. Bouchiat, Phys. Rev. Lett. **64**, 2074 (1990); R. Deblock, R. Bel1, B. Reulet, H. Bouchiat, D. Mailly, Phys. Rev. Lett. **89**, 206803 (2002); V. Chandrasekhar, R. A. Webb, M. Brady, M. B. Ketchen, W. J. Gallagher, A. Kleinasser, Phys. Rev. Lett. **67**, 3578 (1991).
[2] D. Mailly, C. Chapelier, A. Benoit, Phys. Rev. Lett. **70**, 2020 (1993).
[3] V. Ambegaokar, U. Eckern, Phys. Rev. Lett. **65**, 381 (1990).
[4] K. Czajka, M.M. Maska, M. Mierzejewski, Ż. Śledz, Phys. Rev. B **72**, 035320 (2005).

[5] Ho-Fai Cheung, E.K. Riedel, and Y. Gefen, Phys. Rev. Lett. **62**, 587 (1989) and references therein.
[6] Santanu K. Maiti, J. Chowdhury, and S.N. Karmakar, J. Phys.: Cond. Mat., **18**, 5349 (2006); Santanu K. Maiti, J. Chowdhury, S. N. Karmakar, cond-mat/0506390; Santanu K. Maiti, J. Chowdhury, S. N. Karmakar, Synth. Metals, **155**, 430 (2005).
[7] J. Bürki, C. A. Stafford, X. Zotos, and D. Baeriswyl, Phys. Rev. B **60**, 5000 (1999).
[8] See, e.g., E. Cuevas, E. Louis, M. Ortuño, and J.A. Vergés, Phys. Rev. B **56**, 15853 (1997).

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