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Persistent currents in three-dimensional shell-doped nanorings*

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The persistent current in three-dimensional ($P \times N^2$) nanorings as a function of the unit cell number (P), the channel number ($M = N^2$), surface disorder (ξ), and temperature (T) is theoretically investigated in terms of rotational symmetry. On the whole, the typical current increases linearly with $\sqrt{M}$ but decreases exponentially with P, while wide fluctuations exist therein. In the presence of surface disorder, the persistent current decreases with ξ in the regime of weak disorder but increases in the regime of strong disorder. In addition, it is found that the persistent current in perfect rings decreases exponentially with temperature even at $T < T^*$, while in most disorder rings, the typical current decreases slightly with temperature at $T < T^*$.

Keywords: three-dimensional nanorings, tight-binding model, persistent current
PACC: 7335, 7360

1. Introduction

In 1983, Büttiker, Imry, and Landauer suggested the existence, at equilibrium, of persistent currents flowing without dissipation in an isolated one-dimensional (1D) metallic ring threaded by a magnetic flux.[1] These currents result from the quantum interference of the electron wavefunctions, which has been confirmed by experimental observations in single/ensemble isolated mesoscopic rings.[2−8] In ballistic mesoscopic rings (i.e., the mean free path l_e becomes larger than the ring perimeter L), a good agreement between theory and experiment has been reported.[5] In diffusive systems (i.e., $l_e < L$), an open controversy between theory and experiment remains so far. Experimentally, the observed currents are one or two orders larger than all theoretical predictions.[9−16] In addition, the diamagnetic response of the ensemble-averaged persistent current near the zero magnetic fields is contrary to the existing theory.[13,14]

To explore the effect of channels, the theoretical studies mainly focused on two-dimensional (2D) ring models. In the ballistic regime, it was found that the typical current increases with the channel number M as $I_{\rm typ} \sim \sqrt{M}$, while the disorder-averaged current is independent of M,[11,12] only including even Fourier components. Considering the effect of confinement and surface roughness, it has been shown that the typical current increases linearly with the channel number M.[15] In the experiments, however, the line width and line thickness of the rings were usually comparable with its perimeter of length. For example, the sample ring in Jariwala's experiment has a perimeter of length $L \approx 8$ μm, with a line width $w \approx 120$ nm and line thickness $u \approx 60$ nm.[7] This means that a 2D description is oversimplified. Therefore, a three-dimensional (3D) ring model is proposed in this work. It is shown that on the whole, the typical current increases linearly with $\sqrt{M}$ but decreases exponentially with the unit cell number (P), while there exist large fluctuations. The result is at variance with previous theory.

A common view regarding doping in rings is that dopant atoms always suppress the persistent current, in which the dopant atoms are distributed uniformly inside the rings. In the diffusive regime, the typical current is modified by a corrective diffusive factor. In

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the localized regime, the typical current decreases exponentially with disorder.[16] With advances in nanotechnology, actually, the dopant atoms can be spatially confined within a few layers at the nanowire surface.[17] To elucidate the nature of carrier motion in such a system, a shell-doped nanowire model has been proposed.[18,19] It was shown that electrons in a shell-doped nanowire exhibit rather counterintuitive behaviour, namely, the larger the disorder, the weaker the localization. How about the behaviour of the persistent current in a 3D shell-doped-like nanoring? It is a subject of interest in mesoscopic physics.

In experiment, in addition, the temperature is usually very low, so that phonon scattering can be neglected. The effect of temperature on persistent current has been studied by Cheung *et al.*[9] In a linear chain or one-dimensional free electron systems, the persistent current decreases exponentially with temperature at $T > T^*$; however, it is not sensitive to temperature at $T < T^*$. Here, T^* is the characteristic temperature, defined as $T^* = \Delta_{\rm E}/2\pi^2$, where $\Delta_{\rm E} = h v_{\rm f}/L$ is the level spacing at Fermi energy. In the three-dimensional perfect nanoring, interestingly, it was found that the persistent current decreases exponentially with temperature even at $T < T^*$, while in most disorder rings, the typical current decreases slightly at lower temperature $T < T^*$.

2. Model and method

Figure 1 depicts a schematic representation of a shell-doped nanoring. The cross section of the nanoring is a square lattice of size $Na \times Na$, where a is the lattice constant. The perimeter of rings is $L = P \times a$ with $P > N$. Taking a single atomic level per lattice site, the tight-binding Hamiltonian by considering non-interacting electrons is given by[20]

$$H = \sum_i \varepsilon_i c_i^+ c_i + \sum_{i,j} V(i,j) c_i^+ c_j \qquad (1)$$

with on-site energies ε_i, where i labels the coordinates of the sites in the lattice. The hopping integral $V(i,j)$ is restricted to the nearest neighbours of a site. Assuming that the vector potential $\boldsymbol{A}$ has only an azimuthal component, we take $V(i,j) = t\exp(i\int_i^j \boldsymbol{A}{\rm d}\boldsymbol{l})$, in units of the quantum flux Φ_0, where $\boldsymbol{l}$ is a vector that points from the site i to any one of its nearest neighbours. In the present paper, we divide on average the P unit cells into K supercells. In terms of the rotational symmetry, the effective Hamiltonian of a supercell is given by[21]

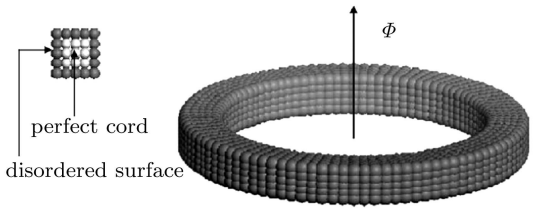


Fig.1. Schematic illustration of a nanoring with surface disorder induced by shell-doping.

$$H_{\rm eff} = H_0 + {\rm e}^{{\rm i}\beta} H_1 + {\rm e}^{-{\rm i}\beta} H_1^+, \qquad (2)$$

where H_0 and H_1 refer to the Hamiltonian matrix in the supercells and the coupling matrix between two neighbouring supercells, respectively. Here $\beta = j \times 2\pi/K$, $(j = 1, 2, 3 \ldots, K)$ is the phase difference between the wave functions of two neighbouring supercells, where K is the number of the supercells contained in the system. For a given β, the eigenlevels can be obtained by diagonalizing the matrix $H_{\rm eff}$. The primitive cell can be doubled and/or trebled in size, forming a supercell. The approach may be efficient and reasonable even in the presence of disorder.

When we neglect interaction of electrons and the self-inductance effect, at zero temperature, the total current of a nanoring can be calculated by the following expression,

$$I_{\rm pc} = -\sum_n \partial E_n/\partial\Phi = -\frac{1}{\Phi_0}\sum_n \frac{\partial E_n}{\partial \phi} \qquad (3)$$

with the summation running up to the last occupied energy level. The current is a periodic function of Φ with fundamental period Φ_0.

At a finite temperature T, the electrons occupy higher levels and all the states participate formally in the total free energy. The total current of a nanoring can be calculated using

$$\begin{aligned} I_{\rm pc} &= -\sum_n \partial f_n/\partial\Phi \\ &= -\sum_n \frac{\partial\left(-k_{\rm B}T\ln\left[1+\exp\left(\dfrac{E_{\rm F}-E_n}{k_{\rm B}T}\right)\right]\right)}{\partial\Phi}, \end{aligned} \qquad (4)$$

where $E_{\rm F}$ is the Fermi energy and $k_{\rm B}$ the Boltzmann constant. Usually, one is interested in the typical current, which is defined as the square root of the disorder

(W) and flux average of the square of the persistent current

$$I_{\rm typ} = \sqrt{\langle I^2 \rangle_{\Phi,W}}. \quad (5)$$

In a three-dimensional shell-doped nanoring, the on-site energies take random values distributed within interval $[-\xi, \xi]$ for the shell (surface) region and the on-site energies are taken to be $E_{\rm F}$ for the core region, ξ describing the degree of the shell disorder introduced by the dopant atoms. The Anderson Hamiltonian includes not only the contribution of the potential difference of dopant atoms but also the contribution of the lattice distortion induced by doping. In order to preserve the rotational symmetry, the disorder is assumed to be distributed identically in each subcell. Although this approximation is somewhat idealized compared with the realistic case, the results can give a qualitative description for the disorder effects. To obtain good statistics, the typical currents are averaged over many realizations of the disorder configurations. In our calculation, the number of the averaged configurations is 100.

3. Calculations and discussion

Figure 2 shows the typical current $I_{\rm typ}$ in three-dimensional perfect rings ($P \times N^2$) as a function of (a) cross size N and (b) unit cell number P (i.e., ring perimeter). For a given ring perimeter ($P = 100$), the change of $I_{\rm typ}$ with $\sqrt{M}$ can be approximately fitted to the form $I_{\rm typ} = 0.265 + 0.193\sqrt{M}$, similar to that in 2D disorder rings ($P \times N \times 1$).[22] However, it is found from Fig.2(a) that there exist large fluctuations in $I_{\rm typ}$ with $\sqrt{M}$, and the larger $\sqrt{M}$, the stronger the fluctuations. From Fig.2(b), $I_{\rm typ}$ damps exponentially with P, and by quality analysis, $I_{\rm typ} = 3.34\exp(-p/75.4) + 0.18$. Similarly, large fluctuations are obtained in $I_{\rm typ}$ with P, of which the amplitude decreases with P increasing. The results are at variance with previous theory.

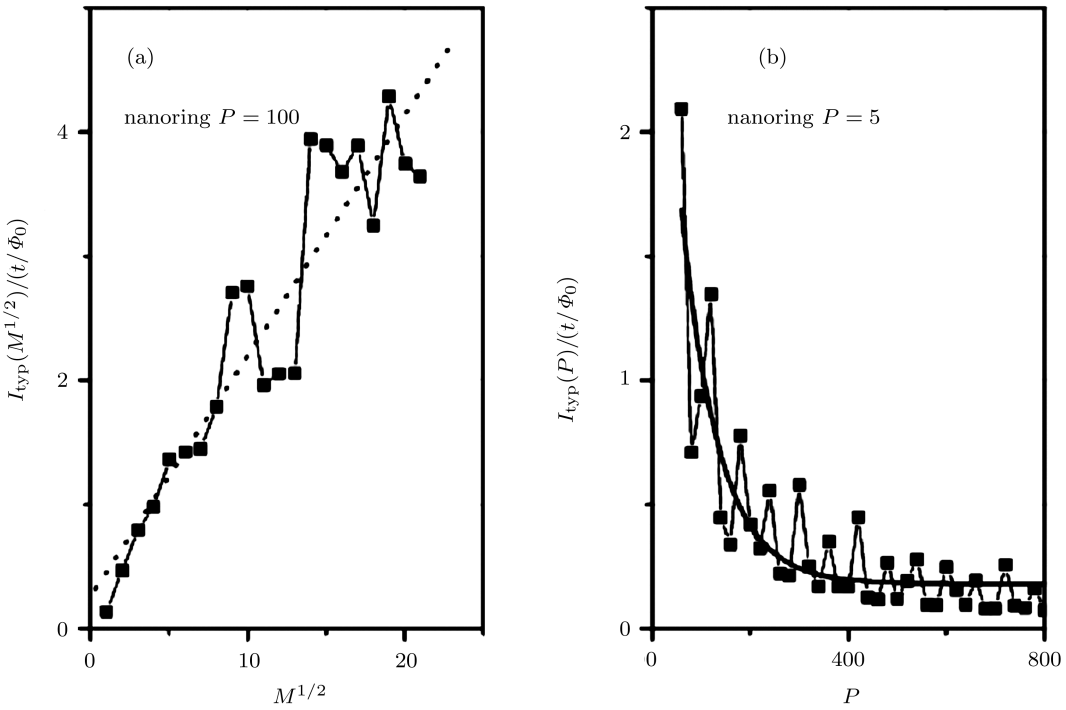


Fig.2. Typical current in perfect rings threaded by magnetic flux, as a function of the channel number $\sqrt{M}$(a) and the unit cells P (b).

To explore the effects of surface disorder, in Fig.3, we calculate $I_{\rm typ}$ as a function of surface disorder. For comparison, the result of $I_{\rm typ}$ versus bulk disorder in the same sample ring is also shown. In the bulk-disordered ring, as expected, $I_{\rm typ}$ decreases with increasing ξ and tends to disappear at $\xi > \xi_{\rm c}$ ($\xi_{\rm c} \approx 4$). This can be easily

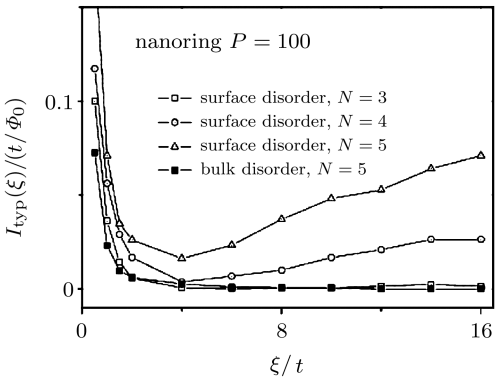


Fig.3. The average typical current in the nanoring of $P = 100$ and $N = 5$ as a function of disorder strength.

understood from the theory of Anderson localization, that is, the larger the disorder, the stronger the localization.[23] The stronger disorder may result in carrier localization, and thus lead to a zero current in the bulk-disordered ring. For the shell-doped nanoring, in Fig.3, we find the overall currents exceed that the in bulk-disordered ring. In particular, $I_{\rm typ}$ exhibits rather counterintuitive behaviour. In the stronger regimes ($\xi > \xi_{\rm c}$), the typical current increases with increasing ξ, while it decreases in the weaker regimes ($\xi < \xi_{\rm c}$). The behaviour is very similar to that in a shell-doped nanowire and order–disorder separated quantum films.[18,19,24] In addition, it is seen from Fig.3 that at given $P = 100$, the typical current increases with increasing N, which is consistent with the case in Fig.2. This further shows that the quantum size effect plays an important role in determining the persistent current in three-dimensional shell-doping nanorings.

To further explore the effect of temperature, Fig.4(a) shows the persistent current versus flux at various temperatures. Here, we assume that the phase coherence length L_ϕ is much larger than L, so that the system remains to be fully described by the eigenfunctions of its Hamiltonian. The effect of temperature is to induce a distribution of the occupancy around $E_{\rm F}$, within $k_{\rm B}T$. The persistent current is given by Eq.(6). For perfect 3D rings, it is seen from Fig.4(a) that T smoothes the sawtooth of the persistent current owing to thermal broadening. With T increasing, the oscillation amplitude of the persistent current declines rapidly. However, T does not destroy the periodicity of the AB oscillation. At a finite temperature, electrons will occupy the states above $E_{\rm F}$. Such states produce the persistent current, the direction of which is opposite to that of the states below $E_{\rm F}$. Therefore, the decrease of the persistent current with T is mainly due to cancellations between the states below and above $E_{\rm F}$. In the presence of surface disorder, Fig.4(b) further shows the typical current versus temperature. For comparison, the result of the perfect 3D ring is also shown. We can see that the typical current

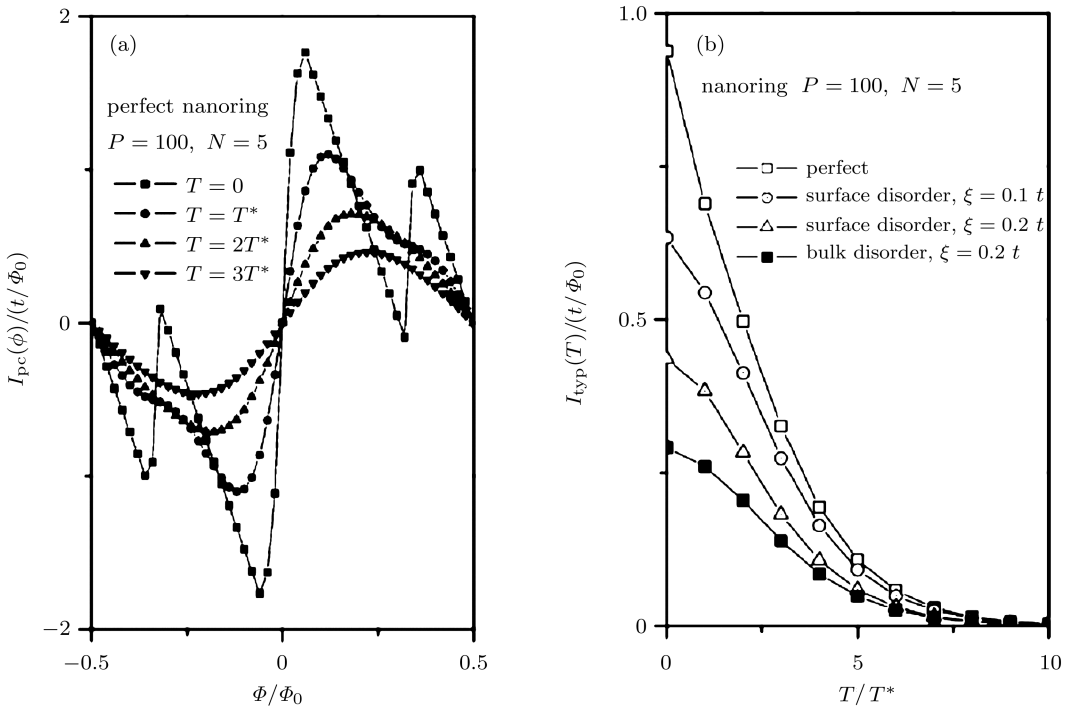


Fig.4. (a) Temperature effect on the persistent current in the three-dimensional perfect nanoring of $P = 100$ and $N = 5$. (b) The average typical currents in nanorings of $P = 100$ and $N = 5$ as a function of temperature T.

of the perfect 3D ring damps exponentially even at $T < T^*$. In the presence of surface disorder, it is shown that at much lower temperatures $T < T^*$, the typical current in disorder rings decreases slightly with temperature. Above $T > T^*$, the typical current is exponentially damped.

4. Summary

In this work, a study of persistent currents in 3D shell-doped nanorings has been presented. In perfect rings, we find that with large fluctuations, the typical current increases linearly with $\sqrt{M}$ and decreases exponentially with P. In the shell-doped ring, nonmonotonic behaviour is observed with increasing surface disorder ξ. The typical current decreases in the regime of weak disorder, while it increases in the regime of stronger disorder. In addition, it is found that the persistent current for perfect rings decreases exponentially with temperature even at $T < T^*$, while in most disorder rings, the typical current decreases slightly with temperature at $T < T^*$. These results have implications for our understanding of the electronic properties and potential applications of 3D nanorings.

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