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Autor: Yang, Xin-E / Zhang, Ling-Yun / Zhou, Yi-Chang

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Inelastic Scattering in a One-Dimensional Mesoscopic Ring at Finite Temperature

By Xin-E Yang

Department of Applied Physics, Tianjin University, Tianjin 300072, China [1]
CCAST (World Laboratory), P. O. Box 8730, Beijing 100080, China

Ling-Yun Zhang

Institute of Physics, Academy of Science, P. O. Box 603-99, Beijing 100080, China

Yi-Chang Zhou

Department of Physics, Zhongshan University, Guangzhou 510275, China

and Jin-Hui Liu

Department of Applied Physics, Tianjin University, Tianjin 300072, China

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Abstract. An expression for the persistent current in the mesoscopic rings considering inelastic scattering between electrons and phonons at finite temperature is derived by variational approach in the tight-binding model. We find that the amplitude of the current is reduced by Debye-Waller factor, the electron-phonon coupling matrix and temperature.[2]

[1] mailing address
[2] PACS numbers: 72.15. Eb, 71.38. +i, 73.20. Dx

Since the Aharonov-Bohm (A-B) effect has been found [1], studies, theoretically and experimentally, have been carried out extensively[2-10]. Especially, the experiments of metallic rings and cylinders stimulate the theoretical research on the persistent currents in mesoscopic systems. Now it has been accepted that the persistent current oscillations result from the quantum interferences of the electron waves in normal-metal rings at low temperature.

Based on the idea that the elastic scattering does not wreck the phase coherence of electrons, Büttiker, Imry and Landauer[11] propose that the change of an external magnetic flux can stimulate the persistent current with the period of $\varphi_0 = hc/e$ called magneton when the loop circumference L is less than the average free path length L_φ of the inelastic scattering of electrons. Under this condition, electrons preserve quantum interferences in the whole ring even when there are a large number of elastic scattering events[12]. Earlier on, in an experiment[13], Sharvin indicated that the A-B effect still occurs in a column sample with 10^4 elastic scattering. It is clarified that the elastic scattering does not destroy electron coherence. From inelastic scattering length $L_\varphi = \sqrt{D\tau_{in}}$, where D is the diffusion coefficient, $\tau_{in} \propto T^{-p}$ (p=constant) is the inelastic scattering time, the temperature should therefore be low enough to make L_φ large enough. Moreover, it is necessary that $L \leq \xi$ (localization length) so that the magnetic field can yield corrections to the boundary conditions of the wavefunctions. In Ref [5], the effect of inelastic scattering has been considered for a ring coupled to an electron-reservoir and for a closed ring, respectively. In the former situation, Büttiker has investigated the effect of the reservoir on the persistent currents in a normal-metal loop and proposed that inelastic processes occurring only in the reservoir are the source of dissipation. For a closed ring, Landauer and Büttiker have discussed the persistent current with inelastic scattering. They have found that inelastic transitions can cause fluctuations in the persistent current, but do not destroy it. Compared to the current at $T = 0$, a small rise in temperature causes only an exponentially small decrease in the persistent current. For dc current, in the absence of inelastic effects the carriers are confined to localized states, and in the presence of intense inelastic scattering, the current flow is impeded by the inelastic scattering. Not long after that, Cheung, Gefen and Riedel[6] performed an analytical calculation for the persistent current in small isolated metal rings. They point out that the amplitude of the persistent current decreases as $exp(-nL/L_\varphi)$ in the strongly disordered regime. This exponential function is the Debye-Waller factor discussed in Ref[14]. In fact, for the inelastic scattering between conduction electrons and phonons, it can be understood that the atoms (pure or impure) in small rings are not static in the sites. In other words, the effects of atomic perturbation to the motion of electrons should not be entirely neglected. The appropriate inelastic scattering are necessary for foundation of thermal equilibrium, though they may disturb more or less the A-B quantum phenomenon.

In this paper, we calculate the persistent currents considering electron-phonon coupling in one-dimensional mesoscopic rings at finite temperature. We assume that the ring is threaded perpendicularly to its own plane by an external magnetic flux φ and that there is no magnetic flux on the circle of the ring with circumference L. By introducing the annihilation and creation operators c_l and c_l^+ of the electron in the lattice site l, the Hamiltonian of the

system is

$$H = H_e + H_{ph} + H_{e-ph}. \tag{1}$$

The Hamiltonian H_e of the electron in the tight-bind model is given by

$$H_e = \sum_l [\varepsilon_0 c_l^+ c_l - J(c_{l+1}^+ c_l + c_l^+ c_{l+1})], \tag{2}$$

where J is the hopping integral and ε_0 is the on-site energy of an electron. The Hamiltonian of the phonon is

$$H_{ph} = \sum_q \hbar\omega_q (n_q + \frac{1}{2}) = \sum_q \hbar\omega_q (b_q^+ b_q + \frac{1}{2}) \tag{3}$$

with the annihilation and creation operators b_q, b_q^+ and the phonon frequency ω_q.

The third term of Eq.(3) is the Hamiltonian for the electron-phonon coupling

$$H_{e-ph} = \sum_q M_q e^{iqla} (b_q + b_{-q}^+) c_l^+ c_l, \tag{4}$$

where M_q is the coupling matrix between the electrons and phonons. To solve the Schrödinger equation $H|\psi>= E|\psi>$, we use the variational method and suppose the variational wave function[14]

$$|\psi>= \frac{1}{\sqrt{N}} \sum_{l=1}^{N} exp[\frac{i2\pi(n+\frac{\varphi}{\varphi_0})}{N}] \quad s_l \quad c_l^+ \quad |\cdots n_q \cdots>, \tag{5}$$

where $|\cdots n_q \cdots>= \prod_q \frac{1}{\sqrt{n_q!}} (b_q^+)^{nq} |0>$ is the phonon state and $s_l = exp[\sum_q f_q e^{ilaq} (b_q - b_{-q}^+)]$ with $f_{-q} = f_{-q}^*$. The variational function (5) is equivalent to the one of LLP theory [15] wave function for a closed mesoscopic ring.

The process of the variational calculation is quite lengthy. To emphasize the feature of the currents motivated by the electron-phonon coupling, we we adopt the approximation of slim energy bands (small J) and of long wave optic phonons ($\hbar\omega_q \sim \hbar\omega_0$). Then, the energy eigenvalues of the Hamiltonian H are calculated as follows

$$E_n = \varepsilon_0 - \sum_q \frac{|M_q|^2}{\hbar\omega_0} - 2Je^{-w} \cos[\frac{2\pi}{N}(n+\frac{\varphi}{\varphi_0})] + \sum_q \hbar\omega_0 (n_q + \frac{1}{2}), \tag{6}$$

where $f_q = M_q/\hbar\omega_0$, $M_q = v(\hbar/2MN\omega_0)^{1/2} iqa$, with the action potential v between the electron and the lattice, and

$$W = \sum_q \frac{2|M_q|^2}{\hbar^2\omega_0^2} \coth \frac{\hbar\omega_0}{2K_B T} [1 - \cos(qa)]. \tag{7}$$

By $I_n = -c\frac{\partial E_n}{\partial \varphi}$, the total current at $T > 0$ is found as

$$I = \sum_n I_n f_n = -\frac{2eJ}{N\hbar} e^{-w} \sum_n \frac{\sin[\frac{2\pi}{N}(n+\frac{\varphi}{\varphi_0})]}{e^{\beta(E_n-\mu)}+1}, \tag{8}$$

where $f_n = 1/[e^{\beta(E_n-\mu)}+1]$ is the Fermi-Dirac distribution of the electrons with the chemical potential μ, $\beta = 1/(K_BT)$. Here, we note that for mesoscopic systems, the canonical and grand-canonical ensembles give rise to different single-level probability distributions. In a canonical ensemble the occupation factors for the electron states are not Fermi functions. However, we can expect that both ensembles give similar results for the persistent current if we consider, for convenience, a system weakly coupled to a particle reservoir. Thus the distribution function is the Fermi-Dirac distribution[6]. Therefore, we adopt a grand-canonical ensemble to calculate the total current. We can expect that the results in a canonical ensemble also exhibit quantum fluctuations with periods φ_0, $\varphi_0/2, \cdots$[8], and that the DWF reduction still appears in the amplitude of the currents. According to the Poisson summation formula $\sum_{n=-\infty}^{\infty} f(n) = \sum_{l=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x)e^{i2l\pi x}dx$ (see Appendix A in Ref.[6]) and by the substitution $k = (2\pi/Na)(x + \varphi/\varphi_0)$ with $N = L/a$, Eq.(10) becomes

$$I = -\frac{eJa^2}{\pi\hbar}e^{-w}\sum_{l=-\infty}^{\infty} e^{-i2\pi l\frac{\varphi}{\varphi_0}}\int_{-\infty}^{\infty}\frac{ke^{ilNka}}{e^{\beta[E(k)-\mu]}+1}dk. \tag{9}$$

The integral in the above equation can be calculated by the Residue Theorem. Thus, the persistent currents for metals and semiconductors are expressed as

$$I = -\frac{4e}{\hbar\beta}\sum_{l=1}^{\infty}\sin\frac{2\pi l\varphi}{\varphi_0}\sum_{n=l}^{\infty}\cos(lNa_1)exp(-lNb_1), \tag{10}$$

where

$$a_1 = \frac{1}{\sqrt{2}}(k_1 + \sqrt{k_1^2 + k_2^2})^{1/2},$$

$$b_1 = \frac{k_2}{2a_1}, \tag{11}$$

$$k_1 = 2 - \frac{(2n-1)\pi\sin W + (A\beta+\alpha)\cos W}{J\beta},$$

$$k_2 = \frac{(2n-1)\pi\cos W - (A\beta+\alpha)\sin W}{J\beta}, \tag{12}$$

$$A = \varepsilon_0 + \sum_q \hbar\omega_0(n_q + \frac{1}{2}) - \frac{|M_q|^2}{\hbar\omega_0},$$

$$\alpha = -\beta\mu.$$

We take the approximation $\sin W \sim W$ and $\cos W \sim 1$ for small W. Then, the total current becomes

$$I = -\frac{2I_0}{\pi}\frac{T}{T_0}\sum_{l=1}^{\infty} exp[-lk_FL\frac{(\mu-A)W}{2\pi E_p}]\sin h^{-1}(l\frac{T}{T_0}\frac{M}{\pi E_p})\sin\frac{2\pi l\varphi}{\varphi_0}\cos(\frac{lk_FL}{\pi}\frac{E_p}{J}), \tag{13}$$

where $I_0 = eV_F/L$, $K_BT_0 = \hbar V_F/(\pi L)$, $E_P = [J(\mu+2J-A)]^{1/2}$, $n_q = 1/[exp(\hbar\omega\beta)-1]$ is the distribution of the phonons. T_0 can be regarded as a mesoscopic characteristic temperature. For $L \sim 2.2 \times 10^{-6}m$, $T_0 \sim 1.5K$.

In order to simplify Eq.(13) we estimate roughly the magnitudes of the parameters ε_0, J, A and μ. Taking $J \sim \varepsilon_0/2$, $\omega_0 \sim 10^{13}sec^{-1}$ and $\varepsilon_0 \sim 5ev$, it can be found that μ, A and J have approximately the same orders of magnitude. Eq.(13), therefore, is simplified as

$$I = -\frac{4I_0}{\pi}\frac{T}{T_0}\sum_{l=1}^{\infty} exp(-lk_FLW)\frac{exp(-lT/T_0)}{1-exp(-2lT/T_0)}\sin(\frac{2\pi l\varphi}{\varphi_0})\cos(lk_FL). \qquad (14)$$

The result above can be regarded as the one for the free-electron model with an electron-phonon coupling at $T > 0$. Comparing the DWF in Eq.(14) with the factor $exp(-nL/L\varphi)$ of Ref.[6], we can clearly see that two functions are consistent with each another.

In summary, we have derived the expression for the total persistent current including the electron-phonon coupling in the tight-binding model. From the expression (13) for the current, we see quite clearly that the current fluctuation is composed of a series of harmonic oscillations with periods $\varphi_0, \varphi_0/2, \ldots$. This is different from the case $T = 0$ where there is only one period φ_0. The major contribution to the persistent current is the first harmonic with $\varphi_0 = hc/e$. The others with $\varphi_0/2, \varphi_0/3, \ldots$ become smaller at increasing order, such that the amplitude of $l = 1$ is about 3 times larger as the $l = 2$ term, and 8.5 times larger as the $l = 3$ term.

We also note that the electron-phonon coupling appears not only in the DWF, but also in the coupling matrix M_q in Eq.(13). This makes the dependence of the currents on the coupling matrix and on the temperature more complicated. However, the DWF still is a very important correction to the current even under low temperature. In fact, it can be understood that at low temperature the number of real phonons is very small. When the temperature rises, the DWF rapidly approaches zero ($W \to \infty$) due to the increasing number of real phonons. In addition, the rising of the temperature also enhances virtual phonon processes. As it is well-known, the DWF coming from an X-ray diffraction experiment depends on the crystal temperature. When the X-rays are scattered by the vibrating lattice atoms, the motion of the atoms partly destroys the phase relationship between the rays contributing to the same diffraction[16]. Actually, we have here is the same situation as in an X-ray experiment. With increasing crystal temperature, the vibrations of the atoms on lattices, deviated strongly from their equilibrium position, become strong. Therefore, the effects of the electron-phonon interaction become strong. That is to say, the inelastic scattering between electron and phonon reduces the amplitude of the persistent current, and with increasing temperature, it will destroy the A-B phase coherence. The DWF is also affected by the coupling coefficient M_q depending on the interaction potential v and on the samples. The experimental choice of the sample can change the value of DWF.

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