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Persistent current in a mesoscopic semiconductor ring with electron–phonon interaction in the two-band model

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Abstract. We have studied, in the framework of the two-band lattice model, the persistent current in a one-dimensional mesoscopic semiconductor ring threaded by a flux ϕ, taking into consideration the electron–phonon interaction at absolute zero temperature. The current is a continuous function and periodic in ϕ, with a flux quantum ϕ_0, without jumps occurring when each period is over. The interband coupling enhances the current while the electron–phonon interaction suppresses it.

1. Introduction

Since the pioneering work of Büttiker *et al* [1, 2], the phenomenon of persistent currents in mesoscopic rings in the presence of magnetic fields has attracted much interest from physicists and experimentalists, who studied it by means of different theoretical models and experimental methods [3–11]. In a normal-metal ring threaded by a magnetic flux, a persistent current was thought to exist as long as the phase coherence of the electron was preserved [1, 2, 4]. By using a gauge transformation, we can remove the vector potential of the magnetic field in the Schrödinger equation with an additional modified boundary condition $\psi_n(x+L) = \exp(2\pi i\phi/\phi_0)\psi_n(x)$, where $\phi_0 = h/e$ is the flux quantum and L is the circumference of the ring. The Bloch wave vector k_n is then determined by a flux-dependent condition, i.e., $k_n = (2\pi/L)(n + \phi/\phi_0)$. Therefore the energy spectrum $\{\varepsilon_n\}$ of the electron is flux dependent and periodic in ϕ, with periodicity ϕ_0. This implies that in thermal equilibrium a current $j = \partial E/\partial\phi$ exists and is periodic in the flux.

Much of the research work has been based on the study of continuous models, without consideration of the effects of the electron–phonon interaction. Zhou *et al* [12] and Wang and Wang [13] studied the persistent current in 1D rings with a lattice model by using different methods. They took the contribution of the electron–phonon interaction into consideration and obtained nearly the same results on the persistent current. Their results show that the oscillation amplitude of the current decreases at a rate governed by a Debye–Waller factor.

We note that almost all of the theoretical models are based on the single-band description, which is suitable only for the simple metallic case. Recently, Wang Yun *et al* [14]

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proposed a continuous two-band model theory for use in studying the persistent currents in semiconductor rings which took into consideration the interband coupling on the basis of the two-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory formulation [15, 16]. They found that the persistent current is periodic in the flux, with the same flux quantum ϕ_0 as in the single-band model, and that the interband coupling enhances the current. However, they did not consider the effects of the electron–phonon interaction in their model. In this paper, the contribution of electron–phonon interaction is taken into consideration in studying the persistent current (at absolute zero temperature) in a 1D mesoscopic electron-doped semiconductor ring threaded by a flux ϕ in the framework of the two-band lattice model.

The paper is organized as follows: in section 2 we present our theoretical model; in section 3 we give some numerical results and analyses; and section 4 gives the conclusions reached using our theory and results.

2. The theoretical model and results

We consider a 1D semiconductor ring with the circumference $L = Na$, where a is the lattice constant and N the number of lattice cells in the ring, lying in the xy-plane, threaded by a magnetic flux ϕ, which can be continuously varied. The Hamiltonian for the 1D mesoscopic semiconductor ring can be constructed in such a way as to include the effect of electron–phonon interaction, on the basis of the two-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory [14–16] in the lattice model from [12, 13] as follows:

$$H = \sum_{l=1}^{N} \begin{pmatrix} \varepsilon_1 c_l^+ c_l - J_1(c_{l+1}^+ c_l + c_l^+ c_{l+1}) & p(c_{l+1}^+ c_l + c_l^+ c_{l+1}) \\ p(c_{l+1}^+ c_l + c_l^+ c_{l+1}) & \varepsilon_2 c_l^+ c_l + J_2(c_{l+1}^+ c_l + c_l^+ c_{l+1}) \end{pmatrix} + \sum_q \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \hbar\omega_q a_q^+ a_q + \sum_{q,l} M_q \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} (\mathrm{e}^{\mathrm{i}qla} a_q + \mathrm{e}^{-\mathrm{i}qla} a_q^+) c_l^+ c_l \tag{1}$$

where $\boldsymbol{q}$ is the wave vector and ω_q is the frequency of the phonon. $\varepsilon_1 = E_c + \varepsilon_{c0}$ and $\varepsilon_2 = E_v - \varepsilon_{v0}$, where E_c and E_v are the edges of the conduction band and valence band respectively, and ε_{c0} (ε_{v0}) and J_1 (J_2), respectively, are the on-site energy and the hopping integral of the conduction (valence) band, which are thought to be independent of l for a perfect lattice. p is a constant parameter, dependent upon the momentum matrix element p_{cv} as in the $\boldsymbol{k}\cdot\boldsymbol{p}$ scheme [14–16]. c_l^+ (c_l) and a_q^+ (a_q) are the creation (annihilation) operators for electrons and phonons respectively. M_q is the coefficient of coupling of the electron and phonon.

Let the state vector $|\psi_n\rangle$ satisfy the Schrödinger equation

$$H|\psi_n\rangle = E_n|\psi_n\rangle. \tag{2}$$

To achieve consistency with the modified boundary condition of the wave function $\Phi_n(x+L) = \exp(2\pi \mathrm{i}\phi/\phi_0)\Phi_n(x)$ [4, 10] in the magnetic field, we set [12, 13]

$$|\psi_n\rangle = \frac{1}{\sqrt{N}} \sum_{l=1}^{N} \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} c_l^+ \mathrm{e}^{2\pi \mathrm{i}(n+\phi/\phi_0)l/N} |A_l\rangle \tag{3}$$

as an approximation for the small-polaron case as in equation (1). In equation (3),

$$|A_l\rangle = \exp\left[\sum_q \left(-\frac{1}{2}|\alpha_q^l|^2 + \alpha_q^l a_q^+\right)\right]|0\rangle \tag{4}$$

is the coherent state of the phonon [13] and satisfies

$$a_q|A_l\rangle = \alpha_q^l|A_l\rangle \tag{5}$$

and $|0\rangle$ is the vacuum state of the electron and phonon. The operators c_l and α_q^l satisfy the following periodic boundary conditions:

$$\alpha_q^{l+N} = \alpha_q^l \tag{6}$$

and

$$c_{l+N} = c_l. \tag{7}$$

Putting the state vector $|\psi_n\rangle$ into Schrödinger equation (2), we get

$$\begin{aligned}
E_n \frac{1}{\sqrt{N}} \sum_l \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} c_l^+ \mathrm{e}^{2\pi \mathrm{i}(n+\phi/\phi_0)l/N} |A_l\rangle
&= \frac{1}{\sqrt{N}} \sum_l \begin{pmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} c_l^+ \mathrm{e}^{2\pi \mathrm{i}(n+\phi/\phi_0)l/N} |A_l\rangle \\
&\quad + \frac{1}{\sqrt{N}} \sum_l \begin{pmatrix} -J_1 & p \\ p & J_2 \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} c_{l+1}^+ \mathrm{e}^{2\pi \mathrm{i}(n+\phi/\phi_0)l/N} |A_l\rangle \\
&\quad + \frac{1}{\sqrt{N}} \sum_l \begin{pmatrix} -J_1 & p \\ p & J_2 \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} c_{l-1}^+ \mathrm{e}^{2\pi \mathrm{i}(n+\phi/\phi_0)l/N} |A_l\rangle \\
&\quad + \frac{1}{\sqrt{N}} \sum_{ql} M_q \alpha_q^l \mathrm{e}^{\mathrm{i}qla} \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} c_l^+ \mathrm{e}^{2\pi \mathrm{i}(n+\phi/\phi_0)l/N} |A_l\rangle \\
&\quad + \frac{1}{\sqrt{N}} \sum_{ql} M_q \mathrm{e}^{-\mathrm{i}qla} \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} a_q^+ c_l^+ \mathrm{e}^{2\pi \mathrm{i}(n+\phi/\phi_0)l/N} |A_l\rangle \\
&\quad + \frac{1}{\sqrt{N}} \sum_{ql} \hbar\omega_q \alpha_q^l \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} a_q^+ c_l^+ \mathrm{e}^{2\pi \mathrm{i}(n+\phi/\phi_0)l/N} |A_l\rangle.
\end{aligned} \tag{8}$$

We see that if the free parameters α_q^l take the following form:

$$\alpha_q^l = -\frac{M_q}{\hbar\omega_q} \mathrm{e}^{-\mathrm{i}qla} \tag{9}$$

the two terms of $a_q^+ c_l^+ |A_l\rangle$ on the right-hand side of equation (8) disappear, and the result will become simple. Multiplying equation (8) on both sides by a conjugate vector $\langle A_l | c_l$, we get

$$\begin{aligned}
E_n \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} &= \begin{pmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} + \begin{pmatrix} -J_1 & p \\ p & J_2 \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} \langle A_l | A_{l-1} \rangle \mathrm{e}^{-\mathrm{i}(2\pi/N)(n+\phi/\phi_0)} \\
&\quad - \left(\sum_q \frac{M_q^2}{\hbar\omega_q} \right) \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} + \begin{pmatrix} -J_1 & p \\ p & J_2 \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} \langle A_l | A_{l+1} \rangle \mathrm{e}^{+\mathrm{i}(2\pi/N}(n+\phi/\phi_0).
\end{aligned} \tag{10}$$

Since the coherent states $|A_l\rangle$ satisfy

$$\langle A_l | A_{l-1} \rangle = \exp\left\{ -\sum_q \left(\frac{M_q}{\hbar\omega_q} \right)^2 (1 - \mathrm{e}^{\mathrm{i}qa}) \right\} \tag{11}$$

and

$$\langle A_l | A_{l+1} \rangle = \exp\left\{ -\sum_q \left(\frac{M_q}{\hbar\omega_q} \right)^2 (1 - \mathrm{e}^{-\mathrm{i}qa}) \right\} \tag{12}$$

equation (10) can be rewritten as

$$E_n\begin{pmatrix}\rho_1\\ \rho_2\end{pmatrix}=\begin{pmatrix}\varepsilon_1 & 0\\ 0 & \varepsilon_2\end{pmatrix}\begin{pmatrix}\rho_1\\ \rho_2\end{pmatrix}+\begin{pmatrix}-J_1 & p\\ p & J_2\end{pmatrix}\begin{pmatrix}\rho_1\\ \rho_2\end{pmatrix}2\mathrm{e}^{-w}\cos\left[\frac{2\pi}{N}\left(n+\frac{\phi}{\phi_0}\right)\right]$$
$$-\left(\sum_q \frac{M_q^2}{\hbar\omega_q}\right)\begin{pmatrix}\rho_1\\ \rho_2\end{pmatrix} \tag{13}$$

where

$$w=\sum_q\left(\frac{M_q}{\hbar\omega_q}\right)^2(1-\cos qa) \tag{14}$$

and in deriving equation (13) we have used the properties of the q-distribution ($-\pi/a \leqslant q < \pi/a$), and the relations $M_{-q}=M_q$ and $\omega_{-q}=\omega_q$. In this case, we have

$$\sum_q\left(\frac{M_q}{\hbar\omega_q}\right)^2\mathrm{e}^{\pm\mathrm{i}qa}=\sum_q\left(\frac{M_q}{\hbar\omega_q}\right)^2\cos qa. \tag{15}$$

Collecting the three terms on the right-hand side of equation (13) together, we obtain

$$E_n\begin{pmatrix}\rho_1\\ \rho_2\end{pmatrix}=\begin{pmatrix}\varepsilon_1-2J_1\mathrm{e}^{-w}C_2-\sum_q\left(\frac{M_q^2}{\hbar\omega_q}\right) & 2p\mathrm{e}^{-w}C_2\\ 2p\mathrm{e}^{-w}C_2 & \varepsilon_2+2J_2\mathrm{e}^{-w}C_2-\sum_q\left(\frac{M_q^2}{\hbar\omega_q}\right)\end{pmatrix}\begin{pmatrix}\rho_1\\ \rho_2\end{pmatrix} \tag{16}$$

where here, and in equation (17) below, C_2 stands for

$$\cos\frac{2\pi}{N}\left(n+\frac{\phi}{\phi_0}\right).$$

Without loss of generality, we may neglect the difference between the effective mass for electrons and light holes [14]. Then we have $\varepsilon_{c0}=\varepsilon_{v0}=\varepsilon_0$ and $J_1=J_2=J$. Solving equation (16), we get the energy spectrum of the modified conduction band:

$$E_n^c=\frac{1}{2}(E_c+E_v)+\frac{1}{2}\sqrt{[\varepsilon_g+2\varepsilon_0-4J\mathrm{e}^{-w}C_2]^2+16p^2\mathrm{e}^{-2w}\cos^2\frac{2\pi}{N}\left(n+\frac{\phi}{\phi_0}\right)} \tag{17}$$

where $\varepsilon_g=E_c-E_v$ is the energy gap between the conduction band and the valence band.

Now we consider an electron-doped semiconductor ring. Each cell has only one conduction electron on average and the valence band is filled with electrons. According to the Pauli exclusion principle, the energy for a fixed N-electron system at absolute zero temperature is (setting $(E_c+E_v)/2$ to be the zero point of energy)

$$E=\frac{1}{2}\sum_{n=-m}^{m-1}\sqrt{\left[\varepsilon_g+2\varepsilon_0-4J\mathrm{e}^{-w}\cos\frac{2\pi}{N}\left(n+\frac{\phi}{\phi_0}\right)\right]^2+16p^2\mathrm{e}^{-2w}\cos^2\frac{2\pi}{N}\left(n+\frac{\phi}{\phi_0}\right)} \tag{18}$$

for $N=2m$, with $m=1,\ 2,\ldots$, and $0\leqslant\phi/\phi_0<1$; and

$$E=\frac{1}{2}\sum_{n=-m}^{m}\sqrt{\left[\varepsilon_g+2\varepsilon_0-4J\mathrm{e}^{-w}\cos\frac{2\pi}{N}\left(n+\frac{\phi}{\phi_0}\right)\right]^2+16p^2\mathrm{e}^{-2w}\cos^2\frac{2\pi}{N}\left(n+\frac{\phi}{\phi_0}\right)} \tag{19}$$

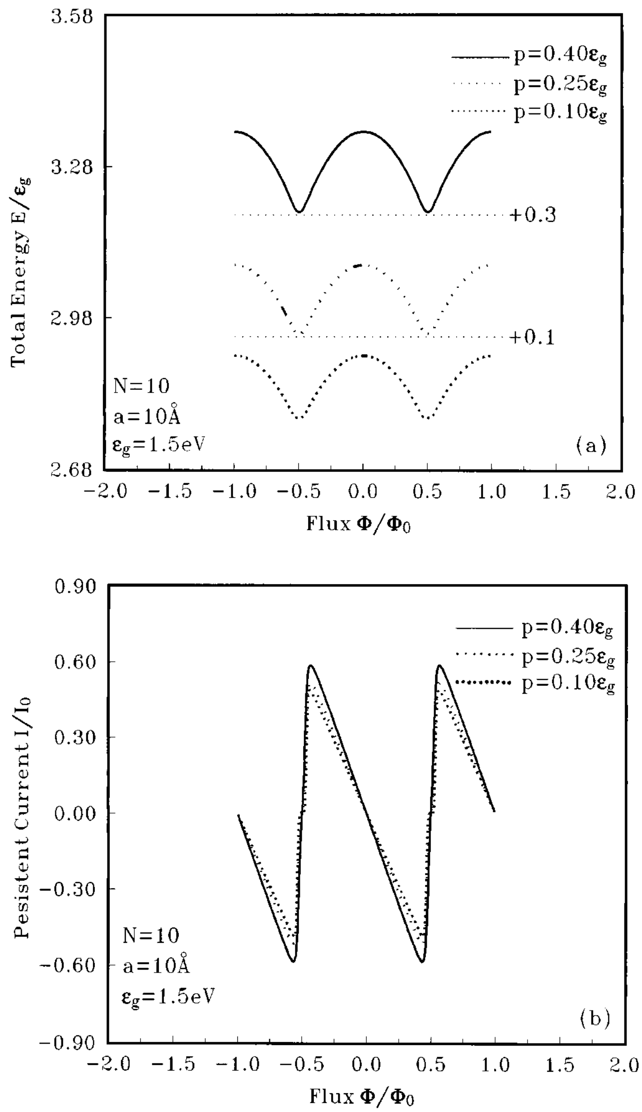

Figure 1. The energy of the electrons (a) and the persistent current (b) versus the magnetic flux ϕ/ϕ_0 for an even number of electrons ($N = 10$). The parameters $\varepsilon_g = 1.5$ eV and $p = 0.1\varepsilon_g, 0.2\varepsilon_g$, and $0.4\varepsilon_g$ are represented by heavy-dotted, light-dotted and solid lines respectively.

for $N = 2m + 1$, with $m = 0, 1, 2, \ldots$, and $-\frac{1}{2} \leqslant \phi/\phi_0 < \frac{1}{2}$. Using the relation [1, 2, 17]

$$I = \frac{\partial E}{\partial \phi} \tag{20}$$

we can obtain the persistent current in the ring.

In order to review the properties of the total energy and persistent current of the semiconductor ring threaded by a magnetic flux, we will perform some numerical analyses in the next section.

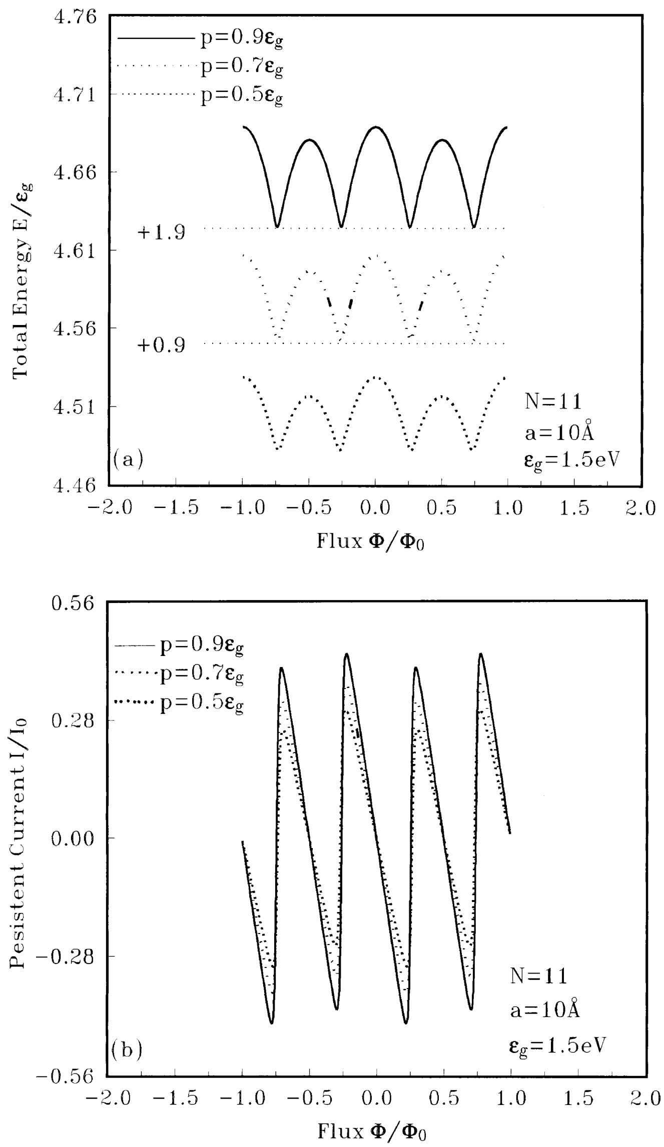

Figure 2. As figure 1, but with $N = 11$ and $p = 0.5\varepsilon_g$, $0.7\varepsilon_g$, and $0.9\varepsilon_g$.

3. Numerical results

In this section, we will give some numerical results to supply more information on the total energy and persistent current for a 1D two-band mesoscopic semiconductor ring with a flux penetrating it.

As in the last section, we neglect the difference between the effective masses of electrons in the conduction band and light holes in the valence band [14]. We set the parameters as follows: $a = 10$ Å, $m = 0.1m_0$, $\alpha = 0.1$, $\hbar\omega_q = \hbar\omega_0 = 30$ meV, and $\varepsilon_g = 1.5$ eV. The energy (E) and the corresponding persistent current (I) are plotted versus the external magnetic flux (ϕ/ϕ_0) in figure 1 for the $N = 10$ system (with $p = 0.1\varepsilon_g$, $0.25\varepsilon_g$, and $0.4\varepsilon_g$), and in figure 2 for the $N = 11$ system (with $p = 0.5\varepsilon_g$, $0.7\varepsilon_g$, and $0.9\varepsilon_g$). In figure 1 and figure 2, the energy and persistent current have been respectively renormalized using the factors ε_g and $I_0 = \varepsilon_g/\phi_0$. At the same time, the energies corresponding to the two larger values of p have been moved down by different amounts so that we can plot them in the same figure.

From figure 1 and figure 2 we know that the energy and persistent current are periodic functions of the flux, with the periodicity of the flux quantum ϕ_0 as in the case of the single-band model for the simple metallic ring. The energy increases as the interband coupling (p) increases, and so does the oscillation magnitude of the persistent current. The persistent current varies abruptly at certain flux points, which are different when the system contains even or odd numbers of electrons. However, this is different from the discontinuous jumps of the persistent current found in the continuous model [14]. The persistent current has one peak for even N and two peaks for odd N in one period of the flux.

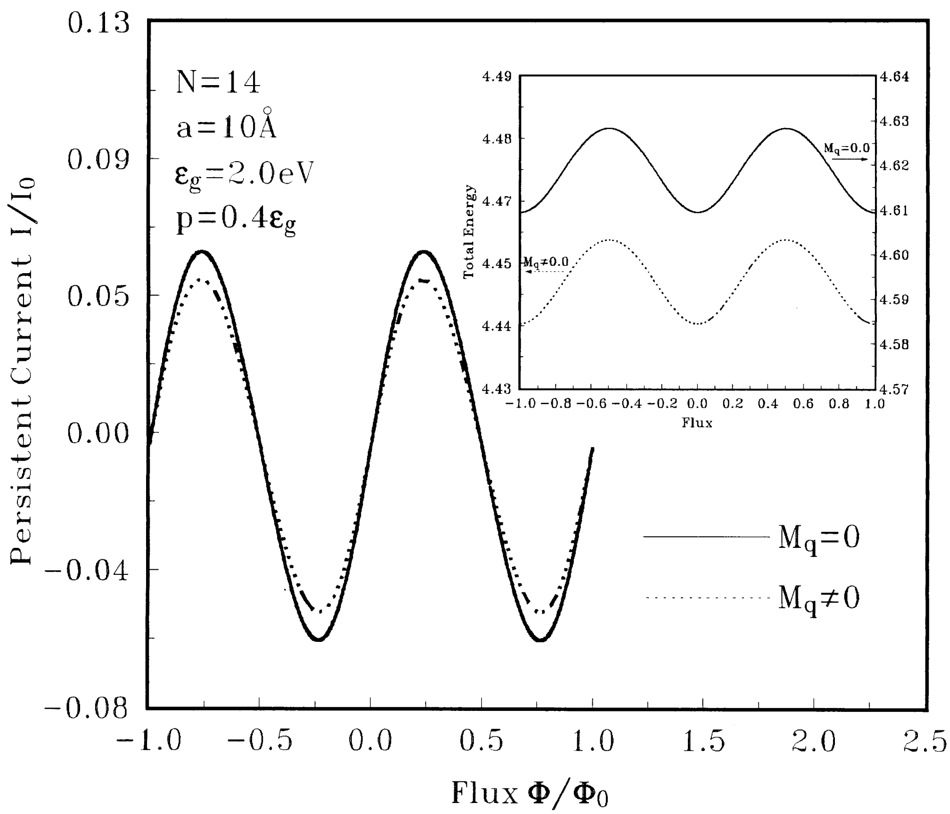

Figure 3. The persistent current versus the magnetic flux ϕ/ϕ_0 for an even numbers of electrons ($N = 14$), and the parameters $\varepsilon_g = 2.0$ eV and $p = 0.4\varepsilon_g$, with (dotted line) and without (solid line) the contribution of electron–phonon interaction.

In figure 3 we have plotted the persistent current for the system with and without the electron–phonon interaction. The inset in the figure shows the system energy in the two cases. The effect of electron–phonon interaction is reflected in the factor e^{-w} in equations (18) and (19), where w is determined by equation (14). Using the same parameters as above, we have $w = 0.005$. We note that the interaction lowers the energy and depresses the persistent current in the system.

4. Conclusion

In this paper we have studied the persistent currents in the 1D mesoscopic semiconductor rings threaded by an external magnetic flux ϕ, in the framework of the two-band lattice model at absolute zero temperature, where the contribution of the electron–phonon interaction has been taken into consideration. From the numerical results, we found that the persistent current of the system is continuous, and is periodic in ϕ, with a flux quantum ϕ_0, without jumps occurring when each period is over, no matter whether the system has even or odd numbers of conduction electrons. This is very different from the situation in the continuous model [14]. We also found that in the semiconductor ring the interband coupling (p) enhances the current while the electron–phonon interaction suppresses the current.

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