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The Aharonov–Casher phase and persistent current in a polyacetylene ring

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Abstract

We investigate a polyacetylene ring in an axially symmetric, static electric field using a modification of the Su–Schrieffer–Heeger (SSH) Hamiltonian for a polyacetylene chain. An effective gauge potential of the single-electron Hamiltonian due to spin–field interaction is obtained and it results in a Fröhlich-type superconductivity equivalent to the effect of a travelling lattice wave. The total energy as well as the persistent current density are shown to be periodic functions of the flux of the gauge field embraced by the polyacetylene ring.

Much attention in the study of mesoscopic systems has been concentrated upon topological effects in multiply connected geometries. As is well known, the Aharonov–Bohm (AB) effect leads to a number of remarkable interference phenomena in mesoscopic systems, especially in a ring [1]. A typical example of the phenomena first observed by Büttiker *et al* is the oscillation of the persistent current in mesoscopic rings threaded by a magnetic flux [1,2] which leads to a relative phase in the wave function of a charged particle due to the U(1) gauge theory. Since the realization of the Berry phase is characterized by a geometric meaning, it has been predicted that analogous interference effects can be induced by the geometric phases which originate from the interplay between an electron's spin and orbital degrees of freedom. Loss *et al* studied the persistent current in a one-dimensional ring in the presence of a static inhomogeneous magnetic field, considering the coupling between spin and orbital motion due to the Zeeman interaction [3]. Using the imaginary-time path-integral method, they showed that the spin wave function accumulates a Berry phase which leads to a persistent equilibrium current [3]. The Aharonov–Casher (AC) effect in mesoscopic systems has also been of great interest, since it specifically includes the spin degree of freedom. Meir *et al* showed that spin–orbit (SO) interaction in one-dimensional rings results in an effective magnetic flux [4]. Mathur and Stone then pointed out that the observable phenomena induced by SO interactions are essentially the manifestation of the AC effect and proposed an experiment to observe the AC oscillation of the conductance in semiconductor samples [5]. Subsequently Balatsky and Altshuler [6] and

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Choi [7] studied the persistent current related to the AC effect. Inspired by these studies on textured rings, various authors have analysed the AC effect in connection with the spin geometric phase. Aronov and Lyanda-Geller considered the spin evolution in conduction rings, and found that SO interaction results in a spin–orbit Berry phase which plays an interesting role in the transmission probability [8]. However, in real systems, the interactions between electrons, lateral dimensions, impurities and the couplings of spins complicate the situation. Cheung *et al* have systematically studied the persistent currents in ideal, one-dimensional metallic rings, including temperature and impurity effects [9]. Experimental observations of persistent currents in an ensemble of $\sim 10^7$ Cu rings [2], in single gold rings [10] and in a single loop in a GaAs heterojunction [11] have also been reported.

It has long been known that the interaction between electrons and the field of lattice displacements may be responsible for superconductivity, known as Fröhlich superconductivity [12]. The average electron momentum corresponds to that of a travelling lattice wave which results in a persistent current in a one-dimensional lattice with a periodic boundary condition, i.e. a ring. The periodic lattice displacement gives rise to an energy gap in the single-electron spectrum with all levels below the gap occupied and all those above it empty. Fröhlich suggested that if, when the electrons were displaced in k-space (see figure 1) so as to give a current flow, the gaps follow the displaced Fermi surface, superconductive behaviour might result, and this is called fluctuation superconductivity or paraconductivity. The existence of the energy gap eliminates the possibility of elastic scattering, provided that the velocity of the travelling lattice wave is sufficiently small. Therefore at low temperature an electric current can exist without resistance. Originally, Fröhlich's mechanism of superconductivity, because of the restriction to one dimension, was regarded as a mathematical model without real physical significance. However, Bardeen pointed out that [13] it was Fröhlich's one-dimensional model rather than a BCS type of pairing that was able to account for the origin of the superconductivity in the experiment of Coleman *et al* [14] who observed an extraordinary increase in conductivity just above the Peierls soft-mode instability in a one-dimensional organic solid. Fröhlich's theory was originally based on a nearly free-electron model and applied only to $T = 0$ K. This concept, i.e. the superconductivity in one-dimensional systems resulting from a coupling between the electrons and a travelling macroscopically occupied lattice wave, was further developed by Allender, Bray and Bardeen [15]. In a superfluid there must be macroscopic occupation of a quantum state that picks out a unique reference frame describing the velocity v_s of the superfluid [15]. Associated with each value of v_s there are a whole set of elementary excitations of the system. When excitations come into equilibrium with the rest frame, a current $j_s(v_s)$ remains. In superfluid helium the macroscopic occupation is the Bose condensate of the momentum state and it is the common momentum of pairs that defines v_s in a superconductor on the basis of pairing. In the Fröhlich model, v_s is determined by the velocity of the macroscopically occupied lattice wave which produces energy gaps at boundaries of the displaced Fermi surface [15] (see figure 1(b)). It was reported in reference [16] that the macroscopic velocity v_s can be induced by the AB magnetic flux in a polyacetylene ring, where the travelling lattice wave is pinned down due to dimerization and the persistent current is solely due to the AB phase which leads to a collective shift of the electron momentum equivalent to that of a travelling lattice wave. Motivated by the formal duality between AB and AC effects (which however have very different physical origins), we in this paper investigate the AC phase which, we will see, also induces persistent current in a polyacetylene ring.

Polyacetylene is the simplest linearly conjugated polymer. The thermodynamically stable *trans*-configuration is sketched in figure 2, illustrating the σ-bonding and the π-bonding in the x–y plane. A tight-binding model is suitable for describing the π-electrons in a polyacetylene

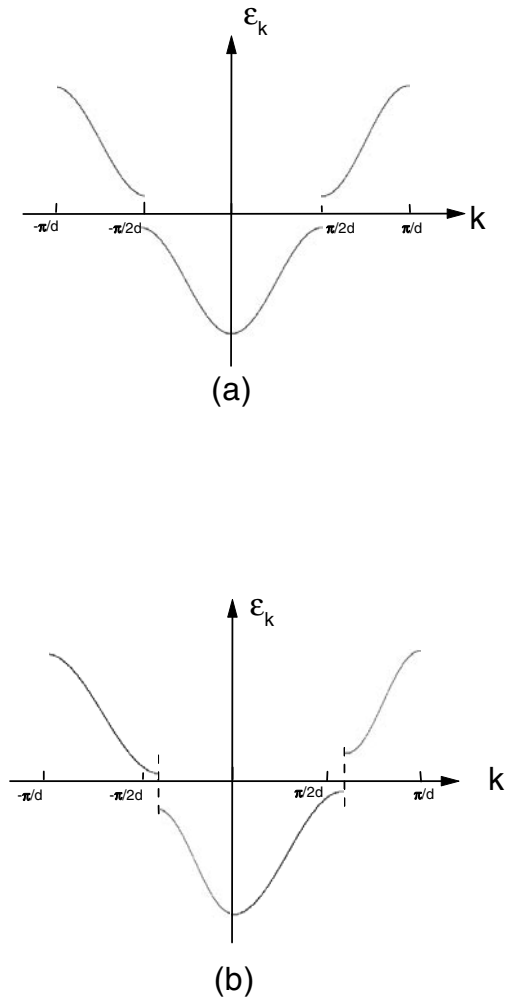

Figure 1. (a) The half-filled tight-binding band which has undergone a Peierls transition. There is no current ($v_s = 0$). (b) As (a), except that $v_s \neq 0$.

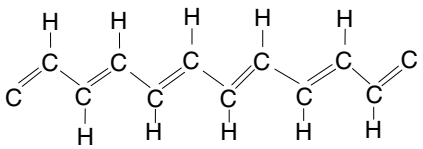

Figure 2. The *trans*-configuration of $(CH)_x$.

chain. A full theory has been given by Su, Schrieffer and Heeger (SSH) [17]. It is certainly interesting to investigate the Fröhlich-like superconductivity related to the AC effect in the context of the modified SSH model. We consider a one-dimensional polyacetylene ring of N electrons in which there is one conduction electron (π-electron) per site, with spacing d. An infinitely long line charge is assumed to be set along the axis of the ring, i.e. the z-axis shown in figure 3. The AC set-up consists of the spin of the π-electron and the electric field of the line

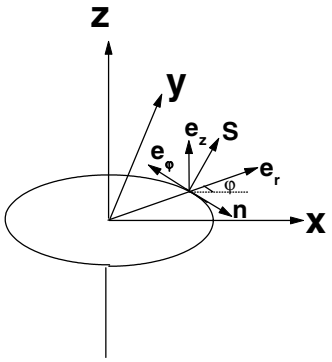

Figure 3. A π-electron with arbitrary polarization of spin $\vec{S}$ in the electric field of a line charge along the z-direction.

charge. The Lagrangian for the π-electron with arbitrary polarization of spin can be written in the nonrelativistic limit as

$$L = \frac{m}{2}\dot{\vec{x}}^2 + \frac{\mu}{c}\dot{\vec{x}} \cdot (\vec{S} \times \vec{E}) - \sum_{n=1}^{N} v(x - R_n) \tag{1}$$

where m and $\vec{x}$ are the mass and position of the electron, respectively. $\vec{E} = E_R \hat{e}_r$ represents the radial static electric field of the line charge with $E_R = 2\rho/R$ where ρ denotes the charge per unit length on the line and R is the radius of the polyacetylene ring. $\mu = g\mu_B$ with $\mu_B = e\hbar/(2mc)$ being the Bohr magneton. g is the spin g-factor which is taken to be 2 here. $\vec{S}$ is then the dimensionless spin operator. $v(x - R_n)$ denotes the potential created by the nth ion with coordinate R_n. The physical significance of the second term in the Lagrangian equation (1) is clear, since a moving magnetic moment $\mu\vec{S}$ is equivalent to an electric dipole moment $(\mu/c)\dot{\vec{x}} \times \vec{S}$. Since we consider a one-dimensional ring, the trivial potential energy of a charged particle in the electric field makes no contribution in the following investigation. The Hamiltonian is

$$h = \frac{1}{2m}\left(\vec{P} - \frac{\mu}{c}\vec{S} \times \vec{E}\right)^2 + \sum_{n=1}^{N} v(x - R_n) \tag{2}$$

where $\vec{P}$ is the momentum. For the π-electron confined on the ring, the Hamiltonian (2) is obtained in cylindrical coordinates as

$$h = \frac{1}{2m}\left(-\mathrm{i}\hbar\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}\varphi} - \frac{\mu}{c}E_R S_z\right)^2 + \left(\frac{\mu}{c}E_R\right)^2 (\vec{n} \cdot \vec{S})^2 + \sum_{n=1}^{N} v(x - R_n) \tag{3}$$

where

$$\vec{n} = (\sin\varphi, -\cos\varphi, 0) \tag{4}$$

is a unit vector shown in figure 3. The azimuthal angle φ is obviously related to the coordinate x by $x = R\varphi$. Considering a tight-binding model with Wannier function ϕ_l per site l such that

$$\left[\frac{\vec{P}^2}{2m} + v(x - R_l)\right]\phi_l = \varepsilon\phi_l \tag{5}$$

we construct the wave function

$$\psi_s(x) = \xi_s \otimes \psi(x) \tag{6}$$

which is the product of the spinor

$$\xi_s = \frac{1}{\sqrt{2}}(|\vec{n}\rangle + |-\vec{n}\rangle) \tag{7}$$

and the spatial wave function

$$\psi(x) = \sum_{l=1}^{N} c_l \phi_l(x). \tag{8}$$

The $|\pm\vec{n}\rangle$ denote the spin coherent states defined by $(\vec{S}\cdot\vec{n})|\pm\vec{n}\rangle = \pm\frac{1}{2}|\pm\vec{n}\rangle$. Taking into account the unit vector $\vec{n}$ expressed in equation (4), we have the spin coherent states written explicitly as

$$\begin{aligned} |\vec{n}\rangle &= \frac{\sqrt{2}}{2}(\mathrm{e}^{-\frac{1}{2}\mathrm{i}\varphi}|+\rangle + \mathrm{e}^{\frac{1}{2}\mathrm{i}\varphi}|-\rangle) \\ |-\vec{n}\rangle &= \frac{\sqrt{2}}{2}(\mathrm{e}^{-\frac{1}{2}\mathrm{i}\varphi}|+\rangle - \mathrm{e}^{\frac{1}{2}\mathrm{i}\varphi}|-\rangle) \end{aligned} \tag{9}$$

where the $|\pm\rangle$ are the usual spin eigenstates of S_z, $S_z|\pm\rangle = \pm\frac{1}{2}|\pm\rangle$.

Averaging over the spin state ξ_s, we obtain the effective Hamiltonian as

$$h_{eff} = \frac{1}{2m}\left(\vec{P} + \frac{e}{c}\vec{A}\right)^2 + \sum_{n=1}^{N} v(x - R_n) \tag{10}$$

where

$$\vec{A} \equiv \frac{c}{2e}\left(\hbar\frac{1}{R} + \frac{\mu}{c}E_R\right)\hat{e}_\varphi$$

is formally equivalent to the vector potential of a magnetic flux with respect to a charged particle with charge e as shown in reference [16]. $\hat{e}_\varphi$ denotes the unit vector in the azimuthal direction. The Hamiltonian operator equation (10) is formally the same as that in reference [16] where the π-electron is in the gauge field of a magnetic flux. We therefore confirm the duality between AB and AC effects by our model study. Following reference [16], we assume that $\psi(x)$ is the eigenfunction of h_{eff}, such that

$$h_{eff}\psi(x) = E(k)\psi(x) \tag{11}$$

and satisfies the usual periodic boundary condition

$$\psi(x + Nd) = \psi(x). \tag{12}$$

Using a unitary transformation

$$\psi'(x) = \exp\left[\mathrm{i}\frac{1}{2\hbar}\left(\hbar\frac{1}{R} + \frac{\mu}{c}E_R\right)x\right]\psi(x) = \exp\left[\mathrm{i}\frac{\Phi_{AC}}{Nd\Phi_0}2\pi x\right]\psi(x) \tag{13}$$

the transformed effective Hamiltonian becomes

$$h'_{eff} = \frac{\vec{P}^2}{2m} + \sum_{n=1}^{N} v(x - R_n) \tag{14}$$

where

$$\Phi_{AC} = \oint \vec{A}\cdot\mathrm{d}\vec{l} = \frac{c}{2e}Nd\left(\hbar\frac{1}{R} + \frac{\mu}{c}E_R\right) \tag{15}$$

is the effective flux of the gauge potential embraced by the ring which we may call the AC flux. $\Phi_0 = ch/e$ is the quantum unit of the flux for a single electron. The stationary schrödinger equation is seen to be

$$h'_{eff}\psi' = E(k)\psi'. \tag{16}$$

The energy eigenvalue $E(k)$ and the eigenfunction $\psi(x)$ are determined by both equation (11) and the usual periodic boundary condition, equation (12). Correspondingly $\psi'(x)$ has a non-trivial boundary condition

$$\psi'(x + Nd) = \exp\left[\mathrm{i}\,2\pi\,\frac{\Phi_{AC}}{\Phi_0}\right]\psi'(x). \tag{17}$$

The vector potential is eliminated in the Hamiltonian h'_{eff} and the energy spectrum $E(k)$ is then determined by equation (16) along with the nontrivial boundary condition of the wavefunction, equation (17). The reason that we make use of the unitary transformation equation (13) to calculate the energy spectrum is that we can thereby adopt Dirac's arguments [18] to demonstrate the periodicity of the spectrum with respect to the magnetic flux following Byers and Yang [19]. The situation is exactly the same as that in the analysis of the magnetic flux quantization in superconductivity. Under the unitary transformation, the kinetic momentum in the Hamiltonian (h_{eff}) equation (10):

$$\vec{P}_{kin} = \vec{P} + \frac{e}{c}\vec{A}$$

becomes

$$\vec{P}'_{kin} = \vec{P}$$

in the Hamiltonian (h'_{eff}) equation (14), where $\vec{P}$ denotes the canonical momentum.

Following the argument of Byers and Yang in their famous paper [19] explaining the magnetic flux quantization in superconductors, we immediately conclude that the eigenvalue $E(k)$ should be a periodic function of the AC flux Φ_{AC} and an even function of Φ_{AC}. When Φ_{AC}/Φ_0 equals an integer, the boundary condition of equation (17) coincides with the usual one, i.e. equation (12), and then the line charge would not lead to any observable effect, similar to the AB case described in reference [16] where the magnetic flux becomes a Dirac string. Using equation (15) it is easy to see that the charge per unit length for the line charge resulting in no observable effect is equal to

$$\rho = \left(n + \frac{1}{2}\right)\frac{mc^2}{e}$$

where n is an integer. The AC partner of the quantum unit of magnetic flux Φ_0 in reference [16], i.e. in the AB case, is seen to be $\rho_0 = mc^2/e$.

To see how the eigenvalue $E(k)$ depends on the AC flux, we evaluate the single-electron energy band with a small variation of the AC flux from integral units of Φ_0. The second-quantization Hamiltonian of the electron can be written as

$$\begin{aligned} H &= \int \psi^{+}(x) h_{eff}\psi(x)\,\mathrm{d}x = \int \psi'^{+}(x) h'_{eff}\psi'(x)\,\mathrm{d}x \\ &= -\sum_l [t_0 - \alpha(u_{l+1} - u_l)](a^{+}_{l+1}a_l + a^{+}_l a_{l+1}) + \mathrm{i}Mv_f \sum_l (a^{+}_{l+1}a_l - a^{+}_l a_{l+1}) \\ &\quad + \frac{1}{2}mv_f^2 \sum_l a^{+}_l a_l. \end{aligned} \tag{18}$$

The first sum is the usual result in the tight-binding approximation and is seen to be the SSH Hamiltonian for electrons. t_0 denotes the hopping integral in the ion equilibrium position, namely the undimerized chain, while α is the electron–phonon coupling constant. The second and the third sum come from the contribution of the AC flux, where

$$M \equiv \mathrm{i}\int \varphi^{*}_{l-1}\vec{P}\varphi_l\,\mathrm{d}x$$

is the dipole matrix element which is assumed to be the same for all l and

$$v_f = \frac{2\hbar\pi}{mNd}\frac{\Phi_{AC}}{\Phi_0}$$

is regarded as a macroscopic velocity of electrons induced by AC flux, i.e.,

$$v_s = v_f.$$

For the perfectly dimerized chain, the displacement configuration of the lattice may be written as $u_n = (-1)^n u$. Following SSH we separate the a_n into those of odd (a_{n_o}) and even (a_{n_e}) indices and introduce the Fourier transforms

$$\begin{aligned} a_{n_o} &= \frac{1}{\sqrt{N}}\sum_k (c_k^v + c_k^c)\mathrm{e}^{-\mathrm{i}\,2\pi n_o kd} \\ a_{n_e} &= \frac{1}{\sqrt{N}}\sum_k (c_k^v - c_k^c)\mathrm{e}^{-\mathrm{i}\,2\pi n_e kd} \end{aligned} \tag{19}$$

where $|k| \leqslant 1/(4d)$; the superscripts v and c denote the valence and conduction bands respectively. The Hamiltonian (10) can be expressed in the k-representation:

$$\begin{aligned} H = &\sum_k E_0(k)(c_k^{v+}c_k^v - c_k^{c+}c_k^c) + \mathrm{i}\sum_k \Delta(k)(c_k^{v+}c_k^c - c_k^{c+}c_k^v) \\ &+ 2v_f M\sum_k \sin(2\pi kd)(c_k^{v+}c_k^c - c_k^{c+}c_k^v) + \frac{1}{2}mv_f^2\sum_k (c_k^{v+}c_k^v + c_k^{c+}c_k^c) \end{aligned} \tag{20}$$

where

$$\begin{aligned} E_0 &= -2t_0\cos(2\pi kd) \\ \Delta(k) &= 4\alpha u\sin(2\pi kd). \end{aligned} \tag{21}$$

In order to diagonalize the Hamiltonian (20), we make the following Bogoliubov transformation:

$$\begin{aligned} a_k^v &= -\mathrm{i}\alpha_k c_k^v + \beta_k c_k^c \\ a_k^c &= \alpha_k^* c_k^v + \mathrm{i}\beta_k c_k^c \end{aligned} \tag{22}$$

with $|\alpha_k|^2 + |\beta_k|^2 = 1$. The diagonalized form is

$$H = -\sum_k E(k)(a_k^{v+}a_k^v - a_k^{c+}a_k^c) + \frac{1}{2}mv_f^2\sum_k (a_k^{v+}a_k^v + a_k^{c+}a_k^c) \tag{23}$$

where

$$\begin{aligned} E(k) &= \sqrt{E_0'(k)^2 + \Delta(k)^2} \\ E_0'(k) &= E_0(k) + 2v_f M\sin 2\pi kd. \end{aligned} \tag{24}$$

A real solution for the transformation coefficient in equation (22) is seen to be

$$\begin{aligned} \alpha_k &= \frac{1}{\sqrt{2}}\sqrt{1 + \frac{E_0'(k)}{E(k)}} \\ \beta_k &= -\frac{1}{\sqrt{2}}\frac{k}{|k|}\sqrt{1 - \frac{E_0'(k)}{E(k)}}. \end{aligned} \tag{25}$$

At zero temperature the valence band is occupied while the conduction band is empty. The total energy is obtained as

$$U = -2\sum_{k=-1/4d}^{1/4d}\sqrt{E_0'(k)^2 + \Delta^2(k)} + \frac{1}{2}Nmv_f^2. \tag{26}$$

Under the condition

$$\frac{v_f M}{t_0} \ll \frac{2\alpha u}{t_0} \ll 1$$

the first term can be approximated up to quadratic dependence on the small variation of the AC flux away from an integer value of Φ_0. Since the flux Φ_{AC} whenever it becomes an integral multiple of Φ_0 will not affect the energy eigenvalue $E(k)$, i.e. v_f vanishes, the total energy would be a minimum, as we see from equation (26). The total energy of the occupied valence band has an infinite number of minima wherever the magnetic flux is an integral multiple of Φ_0. The AC flux dependence of the energy is shown in figure 4.

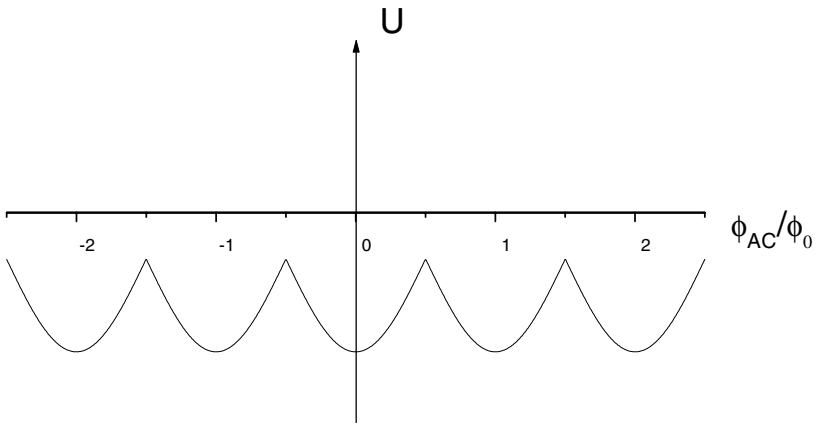

Figure 4. The variation of the total energy as a function of the AC flux.

To obtain the macroscopic momentum shift, namely the displacement of electrons in k-space, we first have to find the electron wave function for the single-electron Hamiltonian h'_{eff}. Such a wave function which leads to the valence band $E_v = -E(k)$ is

$$\psi'(x) = \frac{\exp(\mathrm{i}[mv_f/\hbar]x)}{\sqrt{N}}\left(\alpha_k \sum_n \mathrm{e}^{\mathrm{i}\,2\pi knd}\phi_n + \mathrm{i}\beta_k \sum_n \mathrm{e}^{\mathrm{i}\,2\pi knd}(-1)^n \phi_n\right). \tag{27}$$

The expectation value of the kinetic momentum $\langle \vec{P}_{kin} \rangle$ can be calculated with the above wave function:

$$\langle \vec{P}_{kin} \rangle = \langle \psi | \vec{P} + \frac{e}{c}\vec{A} | \psi \rangle = \langle \psi' | \vec{P} | \psi' \rangle = mv_f + \frac{2ME'_0(k)}{E(k)} \sin(2\pi kd) \tag{28}$$

where the contribution from the second term is negligible when summed over k. The persistent current density due to a small deviation of the AC flux from an integral number of Φ_0 is seen to be

$$j = nev_f \tag{29}$$

where $n = 1/d$ is the electron density. It is seen that the current density depends on the AC flux periodically and is discontinuous at half-integral values of Φ_0, which is shown in figure 5.

In summary, we have studied a polyacetylene ring in the presence of the radial electric field induced by an infinitely long line charge in the one-dimensional tight-binding model with electron–phonon interaction. An effective gauge potential of the π-electron due to spin–field interaction leads to Fröhlich-type superconductivity equivalent to the effect of a travelling lattice wave. The flux of the gauge potential which results in a collective momentum shift of electrons leads to a persistent current, which oscillates with respect to the AC flux and may be observed experimentally with a mesoscopic polyacetylene tube.

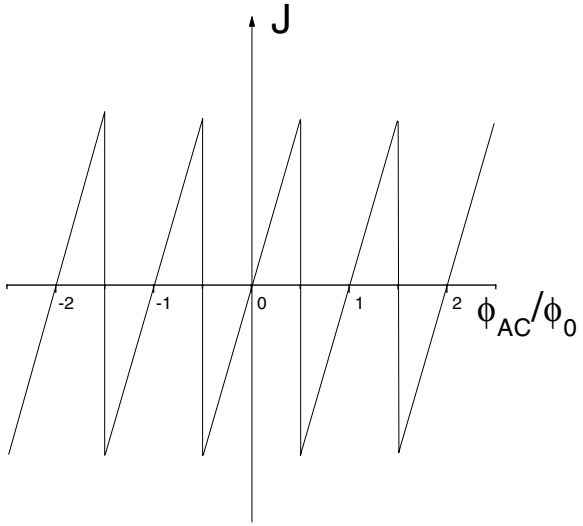

Figure 5. Periodic variation of the current density as a function of the AC flux.

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