Possible persistent current in a ring made of the perfect crystalline insulator

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Abstract

A mesoscopic conducting ring pierced by magnetic flux is known to support the persistent electron current. Here we propose possibility of the persistent current in the ring made of the perfect crystalline insulator. We consider a ring-shaped lattice of one-dimensional “atoms” with a single energy level. We express the Bloch states in the lattice as a linear combination of atomic orbitals. The discrete energy level splits into the energy band which serves as a simple model of the valence band. We show that the insulating ring (with the valence band fully filled by electrons) supports a nonzero persistent current, because each atomic orbital overlaps with its own tail when making one loop around the ring. In the tight-binding limit only the neighboring orbitals overlap. In that limit the persistent current at full filling becomes zero which is a standard result.

Key words: one-dimensional transport, mesoscopic ring, persistent current, coherence

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A mesoscopic conducting ring pierced by magnetic flux \( \phi \) is known to support the equilibrium persistent current. [1,2]. Here we propose possibility of the persistent current in a ring made of the perfect crystalline insulator like for instance the intrinsic silicon crystal. Consider the ring-shaped lattice of one-dimensional (1D) “atoms” in Fig. 1. The electron wave function \( \psi(x) \) in such ring obeys the Schrödinger equation

\[
\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)
\]

with the cyclic boundary condition [1]

\[
\psi(x + L) = \exp(i2\pi\phi/\phi_0)\psi(x),
\]

where \( m \) is the free electron mass, \( x \) is the position along the ring, \( L \) is the ring length, \( \phi_0 = h/e \) is the flux quantum, and \( V(x) \) is the potential of the lattice. The persistent current is

\[
I = -\frac{\partial}{\partial \phi} \sum_n E_n(\phi)/\partial \phi,
\]

where \( \sum_n E_n \) is the ground-state energy of all \( N_e \) electrons in the ring. Solving equation (1) in the lattice model with nearest neighbor hopping one gets [1] for odd \( N_e \)

\[
I = -\frac{4\pi}{N\phi_0} U \sin \frac{N_e}{N} \sin \left(\frac{2\pi \phi}{N\phi_0}\right),
\]

where \( U \) is the hopping amplitude. The persistent current (3) is nonzero in the conductor \( (N_e < N) \) but zero in the insulator \( (N_e = N) \). We want to show that the persistent current is nonzero also in the insulator.

![Fig. 1. Potential \( V(x) \) in a ring-shaped periodic 1D lattice of atoms modelled by one-dimensional potential wells of width \( 2d \) and depth \( V_0 \). The lattice period is \( a \). The ring circumference is \( L = Na \), where \( N \) is the number of atoms.](image-url)
The atomic orbital $\varphi(x)$ and energy $E^{at}$ in a single isolated atom at $x = 0$ obey the Schrödinger equation
\[
\left[ \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + v(x) \right] \varphi(x) = E^{at} \varphi(x),
\]
where $v(x)$ is the atomic potential - the same potential well as in Fig. 1 but with the infinitely thick barriers.

We want to express $\varphi(x)$ via the isolated atomic orbitals. We start with a toy model represented by the "single-atomic" ring in Fig. 2. In the ring geometry
\[
V(x + L) = V(x).
\]
Due to the condition (5), the ring potential $V(x)$ is formally tractable as an infinitely long periodic potential with period $L$ (Fig. 2). Therefore, $V(x)$ can be expressed as an infinite sum of isolated atomic potentials,
\[
V(x) = \sum_{j=-\infty}^{\infty} v(x - jL),
\]
albeit we treat the ring of the finite length $L$, not the infinite crystal. Representation of the infinite crystal allows us to expand $\varphi(x)$ into the atomic orbitals as
\[
\varphi(x) = \sum_{j=-\infty}^{\infty} e^{i(\pi/L)jL} \varphi(x - jL).
\]
Expression (7) can be seen to obey the boundary condition (2) for $k = \frac{2\pi}{L}(\frac{\varphi}{\varphi_0} + n)$, where $n$ is the integer.

We set $k = \frac{2\pi}{L}(\frac{\varphi}{\varphi_0} + n)$ into the equation (7). We get
\[
\varphi(x) = \sum_{j=-\infty}^{\infty} e^{i\frac{2\pi}{\varphi_0}jL} \varphi(x - jL).
\]
We can now evaluate $\langle \psi | \psi \rangle$ as
\[
\langle \psi | \psi \rangle = \int_{-L/2}^{L/2} dx \varphi^*(x) \varphi(x) = \sum_{j=-\infty}^{\infty} \sum_{j'=-\infty}^{\infty} e^{i2\pi \frac{\varphi}{\varphi_0}(j-j')} \int_{-L/2}^{L/2} dx \varphi(x - jL) \varphi(x - j'L) \varphi(x - jL) \varphi(x - j'L)
\]
\[
= \sum_{\Delta L=-\infty}^{\infty} e^{-i2\pi \frac{\varphi}{\varphi_0} \Delta L} \int_{-\infty}^{\infty} dx \varphi(x - \Delta L) \varphi(x),
\]
where the integral in the second line was rewritten as $\int_{-L/2}^{L/2} dx \varphi(x - [j' - j]L) \varphi(x)$, the variables $j$ and $j'$ were changed to the variables $J$ and $\Delta J \equiv j' - j$, and the summation over $j$ was performed.

Further, we write the Hamiltonian in equation (1) in the form $\hat{H} = \hat{H}^{at} + V'(x - jL)$, where
\[
\hat{H}^{at} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + v(x - jL)
\]
Fig. 2. Potential $V(x)$ in the 1D ring with a single 1D atom. The ring circumference $L$ is expanded as a linear cell between $-L/2$ and $L/2$. The cell is then periodically repeated, which is justified by the periodic condition (5).

is the Hamiltonian in (4) for the atom at site $jL$ and
\[
V'(x - jL) = V(x) - v(x - jL).
\]
For the electron energy $E = \langle \psi | \hat{H} | \psi \rangle / \langle \psi | \psi \rangle$ we obtain
\[
E = E^{at} + \frac{1}{\langle \psi | \psi \rangle} \sum_{j=-\infty}^{\infty} \sum_{j'=-\infty}^{\infty} e^{i2\pi \frac{\varphi}{\varphi_0}(j-j')} \int_{-L/2}^{L/2} dx \varphi(x - j'L) V'(x - jL) \varphi(x - j'L),
\]
where we have applied $\hat{H}^{at} \varphi(x - jL) = E^{at} \varphi(x - jL)$. Using similar algebra as in equation (9) we obtain
\[
E = E^{at} - \gamma_0 - \frac{2}{\langle \psi | \psi \rangle} \sum_{\Delta L=1}^{\infty} \gamma_{\Delta L} \cos \left( 2\pi \frac{\varphi}{\varphi_0} \Delta L \right),
\]
where $\gamma_{\Delta L} = -\int_{-\infty}^{\infty} \varphi(x - \Delta L) V'(x) \varphi(x)$ is the overlap integral and we have applied $\gamma_{\Delta L} = \gamma_{-\Delta L}$.

We notice that $\gamma_{\Delta L} \ll \gamma_1$ for $|\Delta L| > 1$ and we also put $\langle \psi | \psi \rangle \simeq 1$. The formula (13) thus reduces to
\[
E = E^{at} - \gamma_0 - 2\gamma_1 \cos \left( 2\pi \frac{\varphi}{\varphi_0} \right).
\]
We set (14) into the expression for the single-electron persistent current, $I = -\partial E(\varphi) / \partial \varphi$. We get
\[
I = -4\pi \frac{\varphi}{\varphi_0} \gamma_1 \sin \left( 2\pi \frac{\varphi}{\varphi_0} \right).
\]
In Fig. 3 we compare the formulae (14) and (15) with the results obtained by solving the equation (1) numerically (the numerical method is described in [3]). Indeed, the formulae (14) and (15) work well. The current (15) is nonzero due to the nonzero overlap integral $\gamma_1$; the atomic orbital overlaps with its own tail making one loop around the ring. In terms of hopping, the electron hops around the ring back into its starting site.

In the multi-atomic ring in Fig. 1 the cyclic condition (2) holds together with the Bloch condition:
\[
\varphi(x + L) = e^{i2\pi \varphi/\varphi_0} \varphi(x), \quad \varphi(x + a) = e^{i\Delta L \varphi} \varphi(x).
\]
The ring potential in Fig. 1 is formally tractable as an infinite lattice potential with period a, given as \( V(x) = \sum_{j=-\infty}^{\infty} v(x - ja) \). This allows to expand \( \psi(x) \)

\[
\psi_k(x) = \sum_{j=-\infty}^{\infty} e^{ikj a} \varphi(x - ja) .
\]

(17)

Expansion (17) obeys the boundary conditions (16) for \( k = \frac{2\pi}{a} \left( \frac{1}{2} + n \right) \), where \( n \) is the integer.

Proceeding in analogy with equation (9) we obtain

\[
\langle \psi_{k_n} | \psi_{k_m} \rangle = \int_{-\infty}^{\infty} dx \psi_{k_n}^*(x) \psi_{k_m}(x) = \\
\sum_{j=-\infty}^{\infty} \sum_{j'=\infty}^{\infty} e^{ik_n(j-j')} \int_{-\infty}^{\infty} dx \varphi(x-j'a) \varphi(x+ja) \\
= N \sum_{\Delta_j=-\infty}^{\infty} e^{-ik_n \Delta_j} \int_{-\infty}^{\infty} dx \varphi(x-\Delta_j a) \varphi(x) ,
\]

(18)

where the integral in the second line was rewritten as

\[
\int_{-\infty}^{\infty} dx \varphi(x-[j'-j]a) \varphi(x) \quad \text{and we summed over } j .
\]

We write the Hamiltonian in equation (1) as \( \hat{H} = \hat{H}_0 + \hat{V}(x - ja) \), where \( \hat{H}_0 = -\frac{\hbar^2}{2m a^2} \frac{d^2}{dx^2} + v(x - ja) \) and \( \hat{V}(x - ja) = V(x) - v(x - ja) \). Using the above relations we express \( E_n = \langle \psi_{k_n} | \hat{H} | \psi_{k_n} \rangle / \langle \psi_{k_n} | \psi_{k_n} \rangle \) as

\[
E_n = E_{nt} + \frac{1}{\langle \psi_{k_n} | \psi_{k_n} \rangle} \sum_{j=-\infty}^{\infty} \sum_{j'=\infty}^{\infty} e^{ik_n(j-j')a} \\
\times \int_{-\infty}^{\infty} dx \varphi(x-j'a) \varphi(x+ja) \varphi(x-j'a),
\]

(19)

where we have applied \( \hat{H}_0 \varphi(x-j'a) = E_n \varphi(x-j'a) \).

Using similar manipulation as in equation (18) and approximating \( \langle \psi_{k_n} | \psi_{k_n} \rangle \simeq N \), we obtain

\[
E_n = E_{nt} - \gamma_0 - 2 \sum_{\Delta_j=1}^{\infty} \gamma_{\Delta_j} \cos (k_n \Delta_j a) ,
\]

(20)

Fig. 3. Ground-state energy and persistent current versus magnetic flux for the “single-atomic” ring from Fig. 2. Two different ring lengths \( L \) are considered. The “atomic” parameters are \( V_0 = 7.03 \text{ eV} \) and \( 2d = 0.14 \text{ nm} \), they give a single atomic level \( E_{nt} = -3 \text{ eV} \). The formulae (14) and (15) (shown in a full line) are compared with the purely numerical approach (shown in a dashed line).

The right panel shows the same results multiplied by \( N^2 \) to estimate the persistent current in a hollow 3D cylinder with cross section of order \( L^2 \) and circumference \( \sim L \). The factor of 1000 appears when 10⁶ cylinders are measured together. Here we have used the parameters \( V_0 = 1.74 \text{ eV}, 2d = 0.01 \text{ nm} \) (giving a single atomic level \( E_{nt} = -0.2 \text{ eV} \)) and two different \( a \).

where \( \gamma_{\Delta_j} = -\int_{-\infty}^{\infty} \varphi(x-\Delta_j a) \hat{V}'(x) \varphi(x) \) is the overlap integral and \( \gamma_{\Delta_j} = \gamma_{\Delta_j} \). Setting (20) into the single-electron current \( I_n = -\partial E_n / \partial \phi \) we obtain

\[
I_n = -\frac{4\pi}{\phi_0} \sum_{\Delta_j=1}^{\infty} \gamma_{\Delta_j} \sin (k_n \Delta_j a) .
\]

(21)

We sum \( I = \sum_n I_n \) over \( n = 0, \pm 1, \pm 2, \cdots (N_e - 1)/2 \) assuming odd \( N_e \) and spinless system. For \( N_e = N \)

\[
I = -(4\pi/\phi_0) N \gamma_N \sin(2\pi \phi/\phi_0) ,
\]

(22)

which the persistent current in the insulating 1D ring. We note that if we keep in (21) only the term with \( \Delta_j = 1 \), the sum \( I = \sum_n I_n \) gives the standard formula (3).

Fig. 4 shows the persistent current (22) as a function of \( L \). It decays with \( L \) exponentially. Enhancement by factor \( \sim N^2 \) can be achieved using the 3D cylinder and by factor of \( 10^5 \) using 10⁶ cylinders on a single chip [2]. But even the largest considered \( L \) is not achievable to present nanotechnology. Due to the 1D atoms, our model is a minimum model. It shows that the persistent current in the insulator exists but it strongly underestimates the effect. For realistic 3D insulators we expect larger persistent currents and technologically feasible sample dimensions. Another possibility is to fabricate the ring-shaped 1D Kronig-Penney model at full filling which also shows the persistent current [4].

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References

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