Instanton Aharonov-Bohm effect and macroscopic quantum coherence in charge-density-wave systems

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It is predicted that in a charge-density-wave (CDW) ring-shaped conductor, placed in an external vector-potential field, there should appear a new Aharonov-Bohm contribution to the magnetic susceptibility and the electrical conductivity oscillating as a function of the flux with the period $\Phi_0=hc/2e$. This contribution arises from instanton transitions between degenerate vacua of the CDW condensate and is the solid-state realization of Θ vacuum in quantum field theory. The period transforms into Φ_0/N in N strongly correlated parallel CDW chains.

The remarkable transport properties of linear-chain conductors such as $NbSe_3$, TaS_3, and $K_{0.3}MoO_3$, as well as of doped linear polymers *trans*-$(CH)_x$ (AsF_5,I,Br), etc., observed at sufficiently low temperatures stimulated considerable research activity in recent years (see reviews[1-3]). These compounds undergo, at moderately low temperature, the Peierls transition to a state which is a condensate of paired electrons and holes differing by the wave vector $2k_F$, the charge-density-wave (CDW) condensate. This macroscopic quantum state is characterized by the complex order parameter, $\Delta\exp(i\phi)$, whose modulus (Δ) defines the energy gap in the single-particle spectrum and the derivatives of the phase (ϕ) provide for the charge and current fluctuations,

$$\delta\rho=\frac{e}{\pi}\frac{\partial\phi}{\partial x},\quad j=-\frac{e}{\pi}\frac{\partial\phi}{\partial t}\ . \tag{1}$$

The above expressions have been derived in the framework of the Fröhlich model of superconductivity.[4] It soon became clear, however, that the various pinning mechanisms of the CDW exclude the existence of supercurrents, but nevertheless the intriguing question remained whether there are any traces of the "superconductivity" in the system. The most direct probe for this hidden superconductivity can be associated with the Aharonov-Bohm effect (flux quantization) in CDW conductors.

Manifestations of flux quantization in solids are displayed by a variety of materials ranging from superconductors to normal metals[5-7] (see review papers[8,9]), where they are associated with the response of free-charge carries to the Aharonov-Bohm flux. The period of conductivity oscillations as well as of nondecaying current oscillations,[7] with respect to the magnetic flux Φ, is $hc/e=4\times10^{-7}$ G cm^2. This effect is mesoscopic, i.e., persists in systems that are large in the atomic scale, but small compared with the electron inelastic mean free path. Weak-localization mechanisms represent another source of conductivity oscillations making their period smaller by half, $\Phi_0=hc/2e$.[10,11] The latter effect is due to the interference in an electron pair, the Cooper pair. Similarly, a realization of the Aharonov-Bohm effect in the magnetic susceptibility oscillations can take place in the absence of free carriers, as discussed in Ref. 12.

In this paper, we consider the collective mechanism of the Aharonov-Bohm effect in Peierls conductors associated with relations (1). Virtual excitations of a CDW condensate are represented by instantons, providing transitions between the degenerate vacua of the CDW and making the energy of the system an oscillating function of the Aharonov-Bohm flux. This phenomenon is generic to the Θ-vacuum problem in the quantum field theory.[13] In our case, the Θ angle is nothing else than the total flux, $\Theta=2\pi\Phi/\Phi_0$. Therefore the subject of the paper has an ideological sense, as it relates the field-theoretical effects to their solid-state realizations.

The Gibbs free energy of a ring-shaped single-chain CDW conductor in the Aharonov-Bohm field, see Fig. 1, is represented as the sum of the modulus and the phase contributions, F_Δ and F_ϕ,[14] of which the latter is of importance in the context of collective Aharonov-Bohm

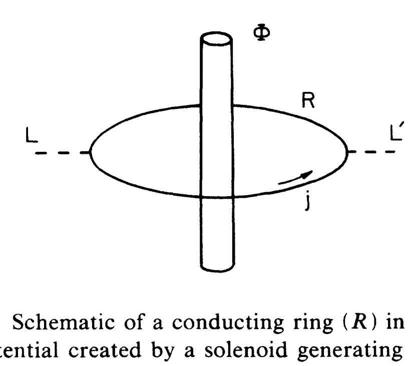

FIG. 1. Schematic of a conducting ring (R) in the field of a vector potential created by a solenoid generating the magnetic flux Φ. In an actual experiment, the flux can be generated by an applied magnetic field, H, and the leads L,L' for measuring resistivity can be attached to the ring. The Aharonov-Bohm effect manifests itself in the appearance of a magnetic moment (persistent current in the appearance of a magnetic moment (persistent current in the ring, j) oscillating, as the ring resistivity, as a function of Φ.

effect. This contribution is expressed as the functional integral:

$$F_\phi = -\frac{1}{\beta}\ln\int D\phi \exp\left[-\int_0^L dx \int_0^\beta d\tau L_E(\phi)\right], \quad (2)$$

where β is the inverse temperature, $\beta = 1/k_B T$, L the ring perimeter, and $L_E(\phi)$ the Euclidean Lagrangian of the CDW

$$L_E(\phi) = N_0[(1/2)\dot{\phi}^2 + (c_0^2/2)(\phi')^2] - (N_0\omega_0^2/M^2)(1-\cos M\phi) - (ie/\pi c)A\dot{\phi}. \quad (3)$$

The last two terms represent the commensurability energy[15] and the interaction of the CDW with the vector potential field A, respectively, and M is the commensurability index subject in the commensurate CDW state to restriction $M \geq 3$. Classical solutions to (3) in the real time $t = i\tau$ are fractionally charged solitons and, in the imaginary time, fractionally charged instantons. The fractional charge is $Q = 2e/M$. In the above expression, $N_0 = 2\Delta^2 N(\varepsilon_F)/\omega^2$, where ω is the renormalized Debye frequency, $c_0 = v_F(\omega/2\Delta) \ll v_F$ the phason propagation velocity ($c_0 \ll v_F$), v_F the Fermi velocity, and $N(\varepsilon_F)$ the electron density of states.

The physics of the instanton Aharonov-Bohm effect is as follows. The phase ϕ is constrained to the condition $0 < \phi < 2\pi$. The quantum-mechanical vacuum-vacuum transition is a combination of the virtual transitions between the eigenstates corresponding to the Lagrangian (3),

$$\Psi_n = |\phi = 2\pi n/M\rangle, \quad n = 0, 1, \ldots, M-1. \quad (4)$$

Each intermediate step $\Psi_n \to \Psi_{n\pm 1}$ acquires a change of the charge equal to the fractional charge $\pm Q$, whereas the net vacuum-vacuum charge transfer equals $\pm 2e$. Thus, the period of the oscillations due to the instanton fluctuations is $(hc/Q)/M = hc/2e$, coinciding with that in superconductors. It can be considered as a manifestation of Fröhlich superconductivity. As the CDW condensate is pinned by the commensurability potential, superconductivity does not show up in an infinite length system but exhibits itself in the periodic variation of the energy with respect to the flux in a simple of a finite length comparable with the phase coherence characteristic scale.[16]

Consider the small size homogeneous system (3) with space gradients omitted and introduce a canonical Hamiltonian operator corresponding to (3):

$$H = (1/2N_0 L)(\hat{P}_\phi + \Phi/\Phi_0)^2 + (N_0\omega_0^2 L/M^2)[1-\cos(M\phi)], \quad (5)$$

where $P_\phi = (h/i)(\partial/\partial\phi)$ is the canonical momentum. The wave function is subject to the periodic condition $\Psi(\phi) = \Psi(\phi + 2\pi)$ which ensures that the formulation (5) is identical to the Bloch problem in a lattice, with $2\pi/M$ substituted for the lattice spacing and Φ for the quasimomentum.[17]

The instantons describe the macroscopic quantum tunneling of the CDW which is easiest for homogeneous trajectories, i.e., for a macroscopic quantum transition of the ring as a whole. Indeed, according to the Derrick theorem (see Ref. 13), there are no space-dependent instanton solutions with a finite action in the Euclidean scalar models in the dimension $d > 1$. Therefore the instanton sine-Gordon solution to (5),

$$\phi(\tau) = (4/M)\tan^{-1}\exp(\omega_0\tau), \quad (6)$$

is advantageous in the action against any inhomogeneous trajectory in a finite volume.

The instanton contribution to the Gibbs energy of CDW at zero temperature is

$$F_{\text{osc}}^{\text{CDW}} = -\lim_{\tau\to\infty}\frac{1}{\tau}\ln\sum_{n=n_-}^{n=n_+}\alpha_n \exp\left[\tau\Delta E\cos\left[\frac{2\pi}{M}(n + \{\Phi/\Phi_0\})\right]\right], \quad (7)$$

where $n_\pm = (\pm M/2 - \{\Phi/\Phi_0\})$, $0 \leq \{\Phi/\Phi_0\} \leq 1/2$; $\alpha_n = 1$ at $n \neq n_\pm$, $\alpha_n = \frac{1}{2}$ at $M/2 \pm \{\Phi/\Phi_0\} = 0, \pm 1, \pm 2, \ldots$, $\alpha_{n_\pm} = 1$ at $M/2 \pm \{\Phi/\Phi_0\} \neq 0, \pm 1, \pm 2, \ldots$; $[x]$ denotes the integral part of x, and $\{x\}$ the periodic function (see Fig. 2),

$$\{x\} = \begin{cases} x - [x] & \text{for } 0 < \{x\} < \frac{1}{2} \\ 1 - x + [x] & \text{for } \frac{1}{2} < \{x\}. \end{cases} \quad (8)$$

The quantity ΔE represents the leading term in the energy splitting of a particle on the circumference due to the instanton transition:

$$\Delta E = 4\hbar\omega_0(S/2\pi\hbar)^{1/2}\exp(-S/\hbar), \quad (9)$$

where $S = 8N_0\omega_0 L/M^2$ is the instanton action calculated at the classical trajectory.

Equation (7) describes the oscillations of the Gibbs energy as a function of Φ with the period Φ_0, at $T=0$. Generalization to finite temperatures is achieved by the

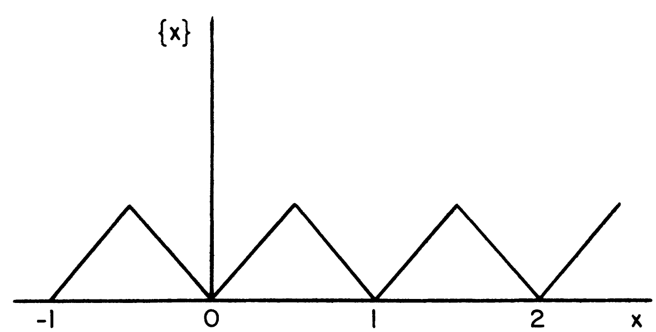

FIG. 2. Graph of $\{x\}$.

β-periodic instanton lattice solution

$$\phi(\tau)=\frac{\pi}{M}\mp\frac{2}{M}\mathrm{am}(\omega_0\tau/\kappa)\ , \tag{10}$$

where $h\omega_0\beta=2\kappa K(\kappa)$, and results in the finite-T action:

$$S_\beta=\frac{S}{\kappa}[E(\kappa)-\tfrac{1}{2}(1-\kappa^2)K(\kappa)]\ , \tag{11}$$

where $K(\kappa)$ and $E(\kappa)$ are elliptic integrals of the first and second kind, respectively. When $\Delta E \ll T \ll \hbar\omega_0$, the temperature dependence of the Gibbs energy is given by the relation $F_{\mathrm{osc}}\sim-(\Delta E)^2/T$. The temperature, at which the instanton contribution to the flux quantization dominates, is about 0.1 K. At higher temperatures, it starts to exponentially decrease. (However, thermally activated solitons should be taken into consideration in this range of temperature.)

To our knowledge, the effect considered is the second known example of quantum phenomena in CDW. The first one was investigated by Bardeen[18] and Maki[19] in an attempt to explain nonlinear CDW conductivity in electric field.

So far we have considered the model of a single chain, an oversimplified version of a practical CDW conductor. To understand the impact of the interchain interaction on the Aharonov-Bohm effect in the CDW, let us first consider the case of two chains. The corresponding Lagrangian is

$$L=\tfrac{1}{2}\dot\phi_1^2+\tfrac{1}{2}\dot\phi_2^2-W[1-\cos(\phi_1-\phi_2)]-\frac{e}{\pi c}A(\dot\phi_1+\dot\phi_2)\ , \tag{12}$$

where W is the magnitude of the interchain interaction (for simplicity, we put here $L=1$, $N_0=1$). The Hamiltonian is

$$H=P_\phi^2+(\hat P_\theta+\Phi/\Phi_0)^2+W(1-\cos\phi)\ , \tag{13}$$

where $\phi=\phi_1-\phi_2$ and $\theta=\phi_1+\phi_2$. The wave function should be periodic in each variable ϕ_1,ϕ_2 with the period 2π which leads to the condition

$$\Psi(\phi,\theta)=\Psi(\phi+2\pi,\ \theta+2\pi)=\Psi(\phi,\ \theta+4\pi)\ . \tag{14}$$

Figure 3 shows the potential profile of the system in the (θ,ϕ) plane. The periodicity $\Psi(\phi,\theta)=\Psi(\phi,\ \theta+4\pi)$ results in the period of the Aharonov-Bohm effect twice smaller than that for a single chain, corresponding to coherent motion of two instantons on both chains, i.e., to the transfer of the charge $4e$ over the ring. However, passing through the barrier W with the probability $\exp(-8W^{1/2})$ will restore the basic period Φ_0.

The above analysis can be easily generalized to the case of an arbitrary number (N) of coupled CDW chains resulting in the Fourier amplitude of the harmonic $\Phi_0/(N-p)$ equal to $\exp[-8W^{1/2}p-S(N-p)]$, where $p=0,1,\ldots,N-1$. The interchain interaction exponentially decreases the amplitude of the basic harmonic with the period Φ_0, so that, in a highly correlated array of chains, only the period $\Phi_N=\Phi_0/N$ survives.

In an experiment, there are always disconnected chains

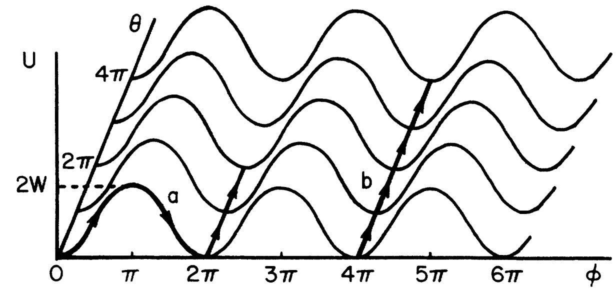

FIG. 3. Potential profile for two interacting incommensurate CDW's. The path a results in an oscillating harmonic with the period Φ_0, whereas the path b corresponds to a harmonic with the period $\Phi_0/2$.

$(q<N)$. This results in that the charge $2qe$ does not participate in the total charge transfer, and the minimum period becomes $\Phi_0/(N-q)$ but the corresponding magnitude does not change. Impurity scattering influences the instanton Aharonov-Bohm effect in a manner different from that for single-particle flux-dependent oscillations.[17] Here, the impurities renormalize the effective phase Lagrangian[20] but do not destroy the quantum coherence.

Dissipation, in turn, can destroy the instanton interference[21,22] but, in the limit of weak inelastic scattering, will only result in a slight modification of the one-instanton action. This problem will be studied in more detail elsewhere.

Thus, we have drawn attention to a new manifestation of the Aharonov-Bohm effect in solids, that of the existence of a nondecaying current (equivalent to the magnetic moment of a ring[7]), the detection of which can prove a useful supplement to the existing observations of the Aharonov-Bohm effect in nonsuperconducting materials. The system considered, the Peierls ring in the field of a vector potential, is a second device, after the small Josephson junction,[22] displaying not only quantum tunneling, but also quantum coherence on the macroscopic scale.

An estimate of the magnitude of the oscillating term in the magnetic moment of a single ring enclosing an area A, $\mu=-A\,\partial E/\partial\Phi$, is at $T=0$ K:

$$\mu_{\mathrm{osc}}\sim A\frac{\hbar\omega}{\Phi_0}(S/2\pi\hbar)^{1/2}\exp(-S/\hbar)\ . \tag{15}$$

The preexponential part of this expression is of the order of $\mu_B A m\omega_0/\hbar$, where $\mu=e\hbar/mc$ is the Bohr magneton and is estimated, for the ring of a perimeter $L\sim10^{-4}$ cm, as $\mu^0_{\mathrm{osc}}\sim10^2\mu_B$. So small moments can, in principle, be detected by superconducting quantum interference device magnetometers.[23,24] To estimate the exponential factor, use the formula for S:

$$S=E_sL/c_0\ , \tag{16}$$

where E_s is the soliton energy, of the order of 1 K, and $c_0\sim10^{6-7}$ cm/s. This follows from the expression $E_s=\alpha\Delta(\Delta/D)^{(M/2)-1}$, where D is the width of the conduction band, and $\alpha\sim1$. For $NbSe_3$ and TaS_3, $M=4$, and

$\Delta/D \sim 0.01$.[1] The same estimate follows from the data on the threshold electric field for nonlinear CDW conduction.[25,26] Therefore, S can be of the order of the action quantum for a ring of the diameter $\sim 10^{-5}$ cm.

The problem of the magnitude is much more serious for a correlated array of chains in crystalline CDW. To make the effect observable, one has to prepare a sample with the number of chains as small as possible. The optimal situation corresponds to N of the order of several tens, i.e., to a submicrometer transverse size of the crystal. Such an experiment should be very difficult.

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