Aharonov–Bohm effect in insulators with a charge-density wave

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The Aharonov–Bohm (AB) effect in Peierls insulators with a charge-density wave (CDW) is investigated. In general the AB effect includes contributions from three mechanisms: one-particle, instanton, and soliton. The one-particle contribution is due to the polarization of the states in a filled energy band by a vector potential field and contributes to oscillations of thermodynamic quantities characterized by a period $\Phi_0 = hc/e$. The instanton contribution is due to macroscopic quantum transitions between degenerate vacuum states of a CDW. The instanton AB effect is considered for the case of an incommensurate CDW and for a commensurate CDW with a commensurability index M. The period of the instanton AB effect is $\Phi_s = \Phi_0/2$. An interchain interaction leads to a fractional base period Φ_s: in a ring consisting of N strongly correlated chains, the base period of the oscillations becomes Φ_s/N. At finite temperatures in a ring consisting of a commensurate CDW there is a contribution of thermally activated solitons, carrying a fractional charge $2e/M$, to oscillations with a period Φ_s.

INTRODUCTION

The Aharonov–Bohm (AB) effect is one of the most thoroughly studied interference phenomena in quantum theory. It combines two of the most important postulates, which are the gauge invariance and the quantum nature of microparticle motion, and it demonstrates the nonlocal nature of the interaction of a charge with an electromagnetic field in a multiply connected region. The AB effect can be detected in condensed media under the conditions of size quantization of the charge-carrier spectrum and is manifested by oscillations of macroscopic characteristics of multiply connected samples observed as a result of a change in a magnetic field flux Φ created by a solenoid (Fig. 1). This effect was first investigated in metals by Kulik[1] who demonstrated that the thermodynamic and transport coefficients include a correction which oscillates as a function of the flux with a fundamental period $\Phi_0 = hc/e$. Under weak localization conditions this oscillation period becomes equal to $\Phi_0/2$ (Ref. 2).[1)]

Until recently it has been assumed that the AB effect can occur only in conductors containing free carriers. In a recent paper by the present authors the effect was extended also to insulators. The new mechanism of the AB effect proposed in Ref. 5 is not related to the motion of free carriers, but is due to the polarization of electron states in the valence band by a vector potential field.

The AB effect in insulators is due to those harmonics of the electron spectrum which are generated by one-particle tunneling between sites separated from one another by distances which are a multiple of L (L is the perimeter of a ring). In wide-gap insulators the amplitude of such a term is negligible, since it is proportional to $\exp(-L/a)$ (a is the interatomic distance). In the case of narrow-gap insulators the number of high harmonics is large because of the strong anharmonicity of the spectrum and their contribution becomes of the order of $\exp(-L\xi_0)$, where $\xi_0 \approx a\varepsilon_v/\Delta \gg a$ (ε_v is the width of the valence band and 2Δ is the gap in the band spectrum).

The AB effect in insulators can be observed in Peierls materials in which the coherence length ξ_0 varies from 10 Å for polyacetylene to several hundreds of angstroms in crystals such as TaS_3, $K_{0.3}MoO_3$, etc.[6,7] The band gap in the latter compounds is a component of the order parameter $\Delta e^{i\varphi}$, the phase φ of which describes the dynamics of a condensate representing a charge-density wave (CDW). A mode φ is electrically active and its gradients give rise to a topological CDW current

$$j_\mu = \frac{e}{\pi} \varepsilon_{\mu\nu}\partial^\nu\varphi, \quad \varepsilon_{\mu\nu} = -\varepsilon_{\nu\mu}, \quad \mu = (t, x), \tag{1}$$

which interacts in the usual (electrodynamic) manner with a vector potential field[8]

$$\mathscr{L}_{int} = j_\mu A^\mu. \tag{2}$$

We can therefore expect a manifestation of the AB effect also in carriers in a collective state such as quantum excitations in a CDW. The AB effect in such systems is investigated below.

In studies of interference phenomena in Peierls–Fröhlich systems we have to distinguish two possibilities. An analog of conduction electrons is a system of real charged excitations in a CDW (phase solitons). Tunnel transitions between lattice sites forming a spectrum of sites in a filled valence band have an analog in the form of virtual excitations known as instantons coupling different energy-degen-

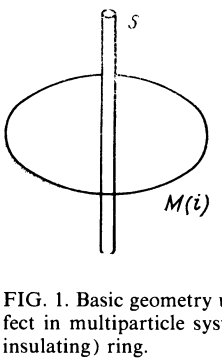

FIG. 1. Basic geometry used in observations of the Aharonov–Bohm effect in multiparticle systems; S is a solenoid and $M(i)$ is a metal (or insulating) ring.

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erate states (vacuum states) of a classical CDW. Such tunneling lifts the degeneracy and in the ring geometry the energy of the ground state of a quantum CDW becomes an oscillatory function of the magnetic flux Φ. However, in contrast to the situation considered earlier in Ref. 5, the tunneling is now macroscopic and not one-particle.

By definition, the phase of a CDW lies within the interval $(0, 2\pi)$. It follows from the Fröhlich relationships given by Eq. (1) that a change in the phase by 2π is equivalent to a change in the charge by $2e$. Therefore, the global 2π symmetry imposes oscillations of the period $\Phi_0/2$ irrespective of the nature of the CDW.

We recall that CDWs are divided into two classes: incommensurate and commensurate. An incommensurate CDW is described by a model of a free zero-mass scalar field φ defined in a finite interval $(0,2\pi)$. A commensurate CDW is described by the sine–Gordon equation and contains a potential energy which is periodic in φ. The commensurability of the lattice imposes an additional period $2\pi/M$ on the potential energy (here, M is the commensurability index which is an integer in the range $M > 2$— see Ref. 9). Therefore, on a circle $(0,2\pi)$ in φ space there are M minima of the CDW potential and the vacuum–vacuum tunneling problem reduces to the problem of a ring with M sites and tunneling between the nearest neighbors. This elementary process corresponds to an instanton connecting the vacuum states

$$\left|\varphi=\frac{2\pi}{M}N\right\rangle \text{ и } \left|\varphi=\frac{2\pi}{M}(N\pm1)\right\rangle$$

(N is an integer) and the tunnel effect then determines the oscillation amplitude. Although each separate instanton $\varphi(\tau)$ carries a fractional "charge"

$$q_f=(e/\pi)\{\varphi(+\infty)-\varphi(-\infty)\}=2e/M$$

and, therefore, the corresponding magnetic flux quantum Φ_f is also fractional, the oscillation period is governed by an M-instanton set and is $\Phi_f = M\Phi_s = MF_0/2$, since only the vacuum states separated by an interval 2π are physically equivalent.

It should be stressed particularly that since the tunneling occurs between quantum states in an insulator ring as a whole, the instanton AB effect represents essentially a manifestation of the macroscopic quantum coherence.[10]

It is useful to study also the relationship between this effect and the topological properties of low-dimensional models of quantum field theory. From this point of view the problem under investigation is similar to the problem of the θ vacuum (see, for example, Ref. 11).

The present paper is organized as follows. A microscopic approach is used in the first section to derive the effective Lagrangian of a Peierls insulator in the form of a ring located in the field of a solenoid. The second section analyzes in detail the incoherent reaction of states in a filled valence band to a vector potential field (AB effect in a narrow-gap insulator). The instanton AB effect is studied in the third section. The fourth section deals with a theory of the AB effect involving thermally excited topological phase solitons carrying a fractional charge. The fifth section is devoted to a theory of the AB effect in an incommensurate CDW. The last (sixth) section deals with the influence of a three-dimensional interaction of chains on the instanton AB effect.

1. MICROSCOPIC MODEL OF A PEIERLS INSULATOR IN THE FORM OF A RING PLACED IN THE FIELD OF A SOLENOID

The microscopic model of a Peierls insulator represents the semiclassical limit of the Hamiltonian of the electron–lattice system (see, for example, Ref. 9). The only difference between the Hamiltonian for a ring placed in the field of a solenoid and the Hamiltonian of a linear chain is the explicit dependence on the vector potential A (Fig. 1):

$$\mathscr{H}=\sum_{n,S} t_{n,n+1}(a_{nS}{}^{+}a_{n+1,S}e^{i\alpha}+\text{H.c.}), \tag{3}$$

where $t_{n,n+1}$ is the integral representing electron transport between the sites in the ring; a_{nS}^{+}, a_{nS}^{-} are the creation and annihilation operators for electrons at a site n characterized by a spin projection S;

$$\alpha=\frac{e}{\hbar c}A(x_{n+1}-x_n),\quad A=\frac{\Phi}{L},\quad L=Na;$$

x_n is the coordinate of a site; N is the number of sites in a ring.

The transition from Eq. (3) to the Hamiltonian of the continuum model is discussed in Ref. 9. In the case of a commensurate one-dimensional Peierls insulator this Hamiltonian is ($\hbar = c = 1$)

$$\begin{aligned}\mathscr{H}=&\psi_S{}^{+}\{iv_F\sigma_3(\partial_x+ieA)+\Delta\sigma_2\exp(-i\sigma_3\varphi)\\&+\mu\Delta\sigma_2\exp[i\sigma_3(M-1)\varphi]\}\psi_S\\&+\frac{\Delta^2}{\lambda}N(0)+\frac{P_\Delta{}^2}{2M_\Delta}+\frac{P_\varphi{}^2}{2M_\varphi},\end{aligned}\tag{4}$$

where λ is the dimensionless electron–phonon interaction constant; $N(0)$ is the density of states at the Fermi level; $P_{\Delta,\varphi}$ are the canonical momenta of the fields Δ and φ;

$$M_\Delta=[\lambda N(0)\,\bar{\omega}^2/2]^{-1},\quad M_\varphi=[\lambda N(0)\,\bar{\omega}^2/2\Delta^2]^{-1};$$

$\bar{\omega}$ is the frequency of phonons with the momentum $2k_F$; σ_i are the Pauli matrices; $\mu \sim (\Delta/\varepsilon_F)^{M-2} \ll 1$; the coordinate x is measured from the ring circle; $x = R\theta$ $(0\leqslant\theta\leqslant2\pi)$; ψ_S is an electron–hole spinor constructed from the operators a_{nS} (Ref. 9). In the case of an incommensurate Peierls insulator the term containing μ is missing.

It is clear from Eq. (4) that the specific nature of the ring geometry is reflected by the presence of a vector potential $A = A_0$, which in the case of a multiply connected space cannot be eliminated by the gauge transformation.

Our task is to calculate the energy of the ground state (at $T=0$) or the free energy (at $T\neq0$). The most convenient calculation method is the representation of a generating functional (partition function) by a functional integral

$$Z=\int D\bar{\psi}_S D\psi_S D\Delta D\varphi\exp\Big(\int_0^L dx\int_0^\beta d\tau\mathscr{L}_E\Big), \tag{5}$$

where $\mathscr{L}_E$ is the Lagrangian in imaginary time $\tau = it$, derived using the Hamiltonian (4), and $\beta = 1/T$.

The integral over the Grassmann variables is easily carried out and the partition function becomes

$$Z=\int D\Delta D\varphi\exp\Big[-\int_0^L dx\int_0^\beta d\tau\mathscr{L}_{eff}(\Delta,\varphi)\Big]$$

$$= \int D\Delta D\varphi \exp\Big(-\int_0^L dx \int_0^\beta d\tau [\mathcal{L}_{eff}(\Delta)+\mathcal{L}_{eff}(\varphi)]\Big), \quad (6)$$

where—according to Ref. 9— we have

$$\int dx\, d\tau \mathcal{L}_{eff}(\Delta)$$

$$=N(0)\int_0^L dx \int_0^\beta d\tau \Big(\frac{\dot{\Delta}^2}{\lambda\overline{\omega}^2}+\frac{\Delta^2}{\lambda}\Big)+\mathrm{Tr}\ln(\gamma_\nu D_\nu - \Delta),$$

$$\gamma_\nu D_\nu = \sigma_2\partial_\tau + v_F\sigma_1(\partial_x + ieA), \quad (7)$$

$$\mathcal{L}_{eff}(\varphi)=N_0\Big[\frac{1}{2}\dot{\varphi}^2+\frac{c_0^2}{2}\varphi'^2+\frac{\omega_0^2}{M^2}(1-\cos M\varphi)\Big]+\frac{ie}{\pi}A\dot{\varphi}. \quad (8)$$

Here,

$$N_0=\frac{2\Delta^2}{\overline{\omega}^2}N(0), \quad c_0=\frac{\overline{\omega}}{2\Delta}v_F, \quad \omega_0=M\overline{\omega}\Big(\frac{\mu}{\lambda}\Big)^{1/2}.$$

The following comments should be made about Eqs. (6)–(8). Separation of the effective Lagrangian into a sum of contributions of each collective degree of freedom $\mathcal{L}_{\text{eff}}(\Delta,\varphi) = \mathcal{L}_{\text{eff}}(\Delta) + \mathcal{L}_{\text{eff}}(\varphi)$ is possible using a parameter such that $\Delta/\varepsilon_F \ll 1$. This parameter allows us to ignore the dependence on the phase in the term $\mathcal{L}_{\text{eff}}(\Delta)$ in a commensurate Peierls insulator. The presence of a second small parameter $\overline{\omega}/\Delta \ll 1$ means that Δ is found from a static extremum $\mathcal{L}_{\text{eff}}(\Delta)$ and $\mathcal{L}_{\text{eff}}(\varphi)$ now contains a self-consistent value $\Delta = \Delta_0$. The square of the gradient φ'^2 and the term representing the interaction of the phase with the vector potential in Eq. (8) appear because of the chiral anomaly effect.[8] The special feature of the multiply connected geometry is that the term $(e/\pi)A\dot{\varphi}$ cannot be eliminated by the gauge transformation even for A = const. For example, if we assume that the field A represents a pure gauge

$$A_\mu=-ig^{-1}\partial_\mu g, \quad g=\exp[i\Lambda(x)], \quad (9)$$

we find from Eq. (1) that

$$\mathcal{L}_{int}=\frac{e}{\pi}\varepsilon^{\mu\nu}A_\mu\partial_\nu\varphi=\frac{e}{\pi}\varepsilon^{\mu\nu}\partial_\mu(\Lambda\partial_\nu\varphi) \quad (10)$$

and the complete Lagrangian is

$$L_{int}=\int dx\mathcal{L}_{int}=\frac{e}{\pi}\int_0^L \partial_x(\Lambda\partial_t\varphi)\,dx$$

$$=\frac{e}{\pi}[\Lambda(L)\dot{\varphi}(L,t)-\Lambda(0)\dot{\varphi}(0,t)]=\frac{e}{\pi}\dot{\varphi}(t)[\Lambda(L)-\Lambda(0)]. \quad (11)$$

On the other hand, we find by definition that

$$\oint A_\mu dx^\mu=\Phi=\oint\frac{\partial\Lambda}{\partial x_\mu}dx^\mu=\Lambda(L)-\Lambda(0), \quad (12)$$

i.e., the quantity $\Lambda(x)$ is a multivalued function in the multiply connected region: $\Lambda(L)\neq\Lambda(0)$ and we have

$$L_{int}=\frac{\Phi}{\Phi_0}\dot{\varphi}. \quad (13)$$

In case of a singly connected space we have $L_{\text{int}}=0$ $[(\Lambda(L)=\Lambda(0)]$.

2. INCOHERENT REACTION OF ELECTRON STATES IN A FILLED VALENCE BAND TO THE FIELD IN A SOLENOID

As pointed out in the Introduction, the AB effect can occur in any insulator even at absolute zero. This general statement is easily justified on the basis of the following elementary considerations.

Let us assume that $\varepsilon(k)$ is the electron spectrum for the valence band such that $\varepsilon(k)=\varepsilon(k+2\pi/a)$. This dispersion law is modified by a vector potential field $\varepsilon(k)\to\varepsilon[k-(e/c)A]$. It should be noted that in the field of a solenoid (curl $A=0$) this is an exact substitution and not a semiclassical one, as in a magnetic field, and it is a direct consequence of the gauge invariance of the theory. The total energy of the filled band in a ring containing N cells is

$$W_{tot}(\Phi)=\sum_{k_n}\varepsilon\Big(k_n-\frac{e}{c}A\Big)=\sum_{n=0}^{N-1}\sum_{m=-\infty}^{\infty}\varepsilon_m$$

$$\times\exp\Big[ima\Big(\frac{2\pi n}{L}-\frac{e}{\hbar c}\frac{\Phi}{L}\Big)\Big]=\sum_{m=-\infty}^{\infty}\varepsilon_m\exp\Big(2\pi im\frac{\Phi}{N\Phi_0}\Big)$$

$$\times\frac{1-\exp(2\pi im)}{1-\exp(2\pi im/N)}=W_0+\sum_{s=1}^{\infty}W_{sN}\exp\Big(-2\pi i\frac{\Phi}{\Phi_0}s\Big). \quad (14)$$

Here, W_0 is the part of the energy independent of the flux Φ and W_s are the amplitudes of the terms oscillating with Φ.

It follows from Eq. (14) that harmonics of the spectrum due to the tunneling of electrons between sites separated by distances which are a multiple of the ring perimeter L oscillate with a period Φ_0 and the amplitude of the oscillations is finite. In the case of a wide-gap insulator when the band gap is $2\Delta\sim\varepsilon_v$, the amplitudes W_s of the oscillations in a macroscopic ring are small: $W_s\propto\exp(-sL/a)$ and the oscillation effect is practically undetectable. The situation is quite different in the case of narrow-gap insulators, which include the Peierls materials. In the case of a Peierls insulator the role of ε_v is played by ε_F and the spectrum of the band states has the relativistic form

$$E(k)=-[\varepsilon^2(k)+\Delta^2]^{1/2}. \quad (15)$$

In view of the anharmonicity of the spectrum the number of higher harmonics is large, of order ε_F/Δ, which gives rise to a strong increase in the amplitude of the oscillatory terms.

The energy of the ground state of a Peierls insulator considered to lowest order in the parameter $\overline{\omega}/\Delta$ corresponds to an extremum of $\mathcal{L}_{\text{eff}}(\Delta)$ of Eq. (7). Routine calculations yield the expression

$$W_\Delta(\Phi)=LN(0)\frac{\Delta^2}{\lambda}-2\sum_{k_n}\Big[v_F^2\Big(k_n-\frac{e}{c}A\Big)^2+\Delta^2\Big]^{1/2}, \quad (16)$$

where $k_n=2\pi n/L$ and the equilibrium value of the gap $\Delta(\Phi)$ is found by minimizing the energy

$$\frac{dW_\Delta(\Phi)}{d\Delta}=0. \quad (17)$$

Separating from Eq. (16) the components oscillating with the period Φ_0, we obtain

$$W_{osc}(\Phi)=\frac{4\Delta}{\pi}\sum_{s=1}^{\infty}\frac{1}{s}K_1\left(\frac{sL}{\xi_0}\right)\cos\left(2\pi s\frac{\Phi}{\Phi_0}-k_FL\right), \quad (18)$$

where $\xi_0=\hbar v_F/\Delta\propto a\varepsilon_F/\Delta$ which is the coherence length of a Peierls insulator; $K_1(x)$ is the modified Bessel function of the second kind of order 1. The expression (18) is meaningful naturally if $L\gtrsim\xi_0$ when the quantum corrections are small and the mean-field approximation can be justified. A phase shift k_FL, which is usually much greater than unity and is typical of the flux quantization effects,[1] is a reflection of the mesoscopic nature of the effect considered in its pure limit.

The equilibrium gap $\Delta(\Phi)$ defined on the basis of the self-consistency equation (17) is given by

$$\Delta(\Phi)\approx\Delta_0\left[1+2\sum_{s=1}^{\infty}K_0\left(\frac{sL}{\xi_0}\right)\cos\left(2\pi s\frac{\Phi}{\Phi_0}-k_FL\right)\right], \quad (19)$$

where $\Delta_0=2\varepsilon_F\exp(-1/\lambda)$ is the order parameter of an infinitely long ($L\to\infty$) Peierls chain; $K_0(x)$ is a modified Bessel function. The nonmonotonic dependence $\Delta(\Phi)$ gives rise to oscillatory corrections to the various characteristics of a Peierls insulator. In particular, in the case of interband absorption of light of frequency $\Omega>2\Delta$ the oscillatory correction to the absorption coefficient is

$$\Gamma_{osc}\approx\frac{64\pi e^2v_F\Delta_0^2n_f}{\Omega^2(\Omega^2-4\Delta_0^2)^{1/2}}\left(1+\frac{2\Delta_0^2}{\Omega^2-4\Delta_0^2}\right)$$
$$\times\sum_{s=1}^{\infty}K_0\left(\frac{sL}{\xi_0}\right)\cos\left(2\pi s\frac{\Phi}{\Phi_0}-k_FL\right). \quad (20)$$

Small oscillatory corrections appear also in the energy of amplitude solitons and polarons in a Peierls insulator (n_f is the two-dimensional density of chains).

The results given in Eqs. (18)–(20) apply to a single chain. In the three-dimensional case if the electron spectrum is represented in the form

$$\varepsilon(k)=\varepsilon_{\parallel}(k_{\parallel})+\varepsilon_{\perp}(k_{\perp}), \quad (21)$$

the quantity W_{osc} should simply be multiplied by the number of chains in a ring. In the case of a spectrum which cannot be described by Eq. (21) the oscillatory behavior is retained, but the amplitude has to be calculated separately in each specific case.

We shall calculate $\Delta(\Phi)$ and W_{osc} at $T=0$. An allowance for the influence of temperature gives rise to exponentially small corrections of the form $\exp(-\Delta/T)\ll1$, since the values of Δ vary from several hundreds of degrees for crystalline Peierls insulators to several thousands of degrees for polyacetylene and the temperature of the Peierls transition is $T_c\ll\Delta$. The temperature effects, however, are important in the instanton AB effect because the characteristic energies of the phase degree of freedom are much smaller that Δ.

3. INSTANTON AHARONOV–BOHM EFFECT IN A COMMENSURATE CHARGE-DENSITY WAVE

We now investigate the phase degree of freedom. The free energy of a charge density wave (CDW) is given by the standard expression

$$F_{CDW}=-\frac{1}{\beta}\ln Z_{CDW}, \quad (22)$$

where

$$Z_{CDW}=\sum_{n=-\infty}^{\infty}\int[D\varphi]_n\exp\left[-\int_0^L dx\int_0^\beta d\tau\mathscr{L}_{eff}(\varphi)\right]. \quad (23)$$

Calculation of the functional integral of Eq. (23) reduces to integration over all the paths satisfying the periodic boundary conditions in terms of the imaginary time $\varphi(\tau)=\varphi(\tau+\beta)$, and additional summation over n, because the paths differing by $2\pi n$ are topologically inequivalent.

The representation (23) is identical with

$$Z_{CDW}=\langle\text{vac}|\exp(-\beta\mathscr{H})|\text{vac}\rangle, \quad (24)$$

where the wave function of the ground state is the direct sum of the wave functions describing homotopically inequivalent vacuum sectors

$$|\text{vac}\rangle\propto\sum_{n=-\infty}^{\infty}|0\rangle_n. \quad (25)$$

We recall that the potential of a commensurate CDW,

$$V_{comm}(\varphi)=\frac{N_0\omega_0^2}{M^2}(1-\cos M\varphi), \quad (26)$$

is subject to (in addition to 2π) $2\pi/M$ periodicity. Therefore, each vacuum–vacuum path ($|0\rangle_n\to|0\rangle_{n\pm1}$) either consists of a sum of one-instanton contributions coupling the nearest minima of the potential (26) (on condition that the total change in the phase is always 2π) or of one M-instanton path directly connecting homotopically inequivalent vacuum states. In the approximation of a low-density instanton gas (see below) the tunnel effect in the M-instanton path is small compared with the one-instanton contribution and can be ignored. We also ignore paths in which instantons and antiinstantons alternate regularly ($|0\rangle_n\to|0\rangle_n$), since they make no contribution to the oscillatory part of the ground-state energy.

We shall consider classical vacuum–vacuum paths $\varphi_c(\tau)$ in imaginary time and small fluctuations of $\delta\varphi$ above them, which leads to a representation of Eq. (23) in the form of a product

$$Z_{CDW}=Z_{ph}Z_t, \quad (27)$$

where

$$Z_{ph}\propto\det{}^{-1/2}(\partial_\tau^2+c_0^2\partial_x^2-\omega_0^2) \quad (28)$$

after regularization gives the partition function of a Bose gas of phasons. Equation (28) follows from Eq. (23) if we allow for small deviations above perturbative vacuum ($\varphi_c^k=2\pi k/M=\text{const}$) and, naturally, it is independent of the magnetic flux. The tunnel partition function Z_t is due to the contribution of large (instanton) fluctuations and in the approximation of low-density instanton gas at $T=0$ it is of the form

$$Z_t=\sum_{\substack{n_i,\bar{n}_i=0\\k=-\infty}}^{\infty}\frac{[8\omega_0\beta(S_0/2\pi)^{1/2}]^{n_i+\bar{n}_i}}{n_i!\bar{n}_i!}\delta_{n_i-\bar{n}_i-kM}$$
$$\times\exp[-n_i(S_0+i\theta)]\exp(-\bar{n}_i(S_0-i\theta)). \quad (29)$$

Here, n_i ($\bar{n}_i$) is the number of instantons (antiinstantons); S_0 is the action calculated for one instanton; $\theta = 2\pi\Phi/\Phi_f$ ($\Phi_f = M\Phi_0/2$ is a flux quantum corresponding to a fractional charge q_f); and the Kronecker delta $\delta_{n_i-\bar{n}_i-kM}$ allows for the circumstance that only the vacuum states separated by an interval 2π are physically equivalent. The numerical coefficient (29) in the preexponential factor in Eq. (12) was calculated first in Ref. 12.

Since the sine–Gordon model has no spatially inhomogeneous instanton solutions, the minimum of the Euclidean action for a chain of length $L \gg (\omega_0/c_0)^{-1}$ is reached for spatially homogeneous solutions.[2)]

$$\varphi_c(\tau) = (4/M)\,\mathrm{arctg}\,\exp(\pm\omega_0\tau) \tag{30}$$

(the $\pm$ signs correspond to an instanton and an antiinstanton). In this case the one-instanton action S_0 describing the macrotunneling of quantum states of a ring as a whole is

$$S_0 = E_s L/c_0 = 8N_0\omega_0 L/M^2, \tag{31}$$

where E_s is the energy of a phase soliton.[13]

If the Kronecker δ is represented in the integral form

$$\delta_{n_i-\bar{n}_i-kM} = \frac{1}{2\pi}\int_0^{2\pi} d\theta \exp[-i\theta(n_i-\bar{n}_i-kM)] \tag{32}$$

and the necessary summation is carried out in Eq. (29), the final result is

$$Z_t = \frac{1}{M^2}\sum_{n=n_-}^{n_+} \alpha_n \exp\left[\beta\Delta E\cos\left(\frac{2\pi}{M}\left(n+\left\{\frac{\Phi}{\Phi_s}\right\}\right)\right)\right]. \tag{33}$$

Here, $n_\pm = [\pm M/2 - \{\Phi/\Phi_s\}]$; $[\ldots]$ indicates the integral part of a number; $\{\ldots\}$ is the distance to the nearest integer; $\Phi_s = \Phi_0/2$ is a "superconducting" flux quantum; and the coefficients α_n are $\alpha_n = 1$ for $n \neq n_\pm$, $\alpha_{n_\pm} = 1/2$ if $M/2 \mp \{\Phi/\Phi_s\}$ is an integer, but $\alpha_{n_\pm} = 1$ otherwise;

$$\Delta E = 4\omega_0(S_0/2\pi)^{1/2}e^{-S_0}. \tag{34}$$

Equation (33) is identical with the generating functional for the energy of a particle in a periodic lattice containing M sites and characterized by a dispersion law obtained in the tight-binding approximation:

$$E(k) = \varepsilon_0\cos(ak_n), \tag{35}$$

where

$$\varepsilon_0 = -\Delta E, \quad a = 2\pi/M, \quad k_n = n + \{\Phi/\Phi_s\}.$$

This analogy is followed in a consistent manner in the Hamiltonian formulation of the problem (see below).

We can thus see that at $T = 0$ the energy of the ground state of a CDW oscillates along a flux characterized by a quantum Φ_s

$$E_0 = -\Delta E\cos\left[\frac{2\pi}{M}\left(n^* + \left\{\frac{\Phi}{\Phi_s}\right\}\right)\right], \tag{36}$$

where n^* is the value for which the argument of the exponential function in Eq. (33) is a maximum. We can easily show that $n^* = 0$ holds if the fractional part of the ratio of the fluxes occurs in the cosine.

Since the term $(e/\pi)A\dot{\varphi}$ represents the total derivative, it does not alter the equation of motion of a CDW, but occurs in the integral characteristics, particularly in the ground-state energy of our quantum problem. Therefore, the interaction with the flux is a topological property of a CDW and the parameter θ in Eq. (29) governs the properties of the θ vacuum, as in the gauge models used in quantum field theory. It should be pointed out also that formally if $M = 1$ holds, then our problem is fully equivalent to that of the quantum pendulum with a θ vacuum state discussed in detail in the literature (see, for example, Ref. 11). The influence of temperature on the oscillations can be allowed for by calculating the action for a periodic (in imaginary time) path

$$\varphi(\tau+\beta) - \varphi(\tau) = 0 \pmod{2\pi}.$$

As at $T = 0$, a minimum of the action occurs for the simplest paths of the type

$$\varphi_c(\tau+\beta) - \varphi_c(\tau) = 2\pi n/M,$$

and 2π periodicity is ensured by an addition: the difference between τ-periodic instantons and antiinstantons (in field theory they are called colorons) is kM ($k = 0, \pm 1, \ldots$). Then, calculation of the low-temperature partition function reduces the replacement of the one-instanton action S_0 by the one-coloron action S_β in Eq. (29). We shall restrict our calculation to just the exponential factor in the tunnel shift of the ground-state energy.

The sine–Gordon equation has explicit spatially homogeneous coloron solutions:

$$\varphi_c(\tau) = \frac{\pi}{M} + \frac{2}{M}\,\mathrm{am}\left(\frac{\omega_0\tau}{\varkappa}\right), \tag{37}$$

where $\mathrm{am}(x)$ is the elliptic amplitude and the period β is related to the elliptic modulus $\varkappa$ by

$$2\varkappa K(\varkappa) = \omega_0\beta, \tag{38}$$

where $K(\varkappa)$ is a complete elliptic integral of the first kind.

The solution (37) describes an instanton crystal with repulsion. Its energy (action) in one period increases on reduction in the crystal period (increase in temperature). These qualitative discussions are sufficient and show that temperature suppresses instantons and their contribution to the energy of the θ vacuum should decrease with temperature.

Using Eqs. (37) and (38), we can readily find the one-coloron action

$$S_\beta = \frac{E_s}{T_C}\Phi(\varkappa), \tag{39}$$

$$\Phi(\varkappa) = \frac{1}{\varkappa}\left[E(\varkappa) - \frac{1}{2}(1-\varkappa^2)K(\varkappa)\right] \tag{40}$$

$$= \begin{cases} 1+4e^{-\omega_0/T}, & T \ll \omega_0, \\ \pi^2 T/4\omega_0, & T \gg \omega_0, \end{cases} \tag{41}$$

where $T_C = c_0/L$ is the characteristic quantum (Casimir) temperature.

The nature of the temperature dependence $S_\beta(T)$ can be understood on the basis of the following quantitative considerations. If $T \ll \omega_0$, the characteristic separation between the instantons T^{-1} is considerably larger than their dimensions ω_0^{-1}. Only the "tails" of the instantons intersect and the interaction (repulsion) is exponentially small. In the opposite limit $T \gg \omega_0$ the potential energy of instantons ($\sim \omega_0$) can be ignored completely. Since the spatial length of an instanton is of the order of L (homogeneous tunneling) and in imaginary time we have $\beta = T^{-1}$, the one-coloron action is

$$S_\beta \sim \iint dx\, d\tau \dot{\varphi}^2 \sim LT, \qquad T \gg \omega_0.$$

In reality the high-temperature asymptotic form of (41) is completely unrelated to the real temperature dependence of the amplitude of oscillations of a commensurate CDW. We have seen already that the tunneling results in an M-fold splitting of the ground-state level of perturbative vacuum with an energy scale of the order of

$$\Delta E \sim \cos\left(\frac{2\pi}{M}\right) \omega_0 S_0^{1/2} e^{-S_0}. \tag{42}$$

Therefore, at temperatures $T \gg \Delta E$ we find that even in the limit $T \ll \omega_0$ the expression for the partition function (33) still contains all M levels of the tunnel energy band. We can easily see that because of interference between the oscillation phases the part of the free energy dependent on the flux Φ then becomes smaller by an additional factor $\sim \Delta E/T$. In the next section we shall see that $T_c \sim \Delta E$ is the true temperature at which the macroscopic quantum coherence is destroyed. However, the high-temperature limit of Eq. (41) is related directly to the real temperature dependence of oscillations of an incommensurate CDW (see Sec. 5).

We conclude this section by providing a Hamiltonian picture of oscillations of a CDW. All the results obtained at $T = 0$ are readily interpreted in terms of the effective Schrödinger equation for a φ particle. The Hamiltonian corresponding to the Lagrangian $L\mathscr{L}_{\text{eff}}$ is

$$H = \frac{L}{2N_0}\left(\frac{\hat{P}_\varphi}{L} + \frac{e}{\pi c}A\right)^2 + \frac{LN_0}{M^2}\omega_0^2(1-\cos M\varphi), \tag{43}$$

where $\hat{P}_\varphi = -i\partial/\partial\varphi$.

The energy levels are found from the Schrödinger equation

$$H\psi = E\psi \tag{44}$$

subject to the boundary condition $\psi(0) = \psi(2\pi)$. Our problem is fully analogous to the Bloch problem in which the role of the quasimomentum is played by the flux Φ (Ref. 13). The wave function $\psi(\varphi)$ is quasiperiodic if we shift it by one period of the potential:

$$\psi\left(\varphi + \frac{2\pi}{M}\right) = \exp\left(iq\frac{2\pi}{M}\right)\psi(\varphi), \tag{45}$$

so that when it is enclosed in the ring the quantity q becomes quantized ($q = m$, where m is an integer). The function $\psi(\varphi)$ can be sought in the form

$$\psi(\varphi) = \exp(i\Phi/\Phi_s)\chi(\varphi), \tag{46}$$

where $\chi(\varphi)$ satisfies the Mathieu equation.

The explicit dependence of the spectrum on the flux Φ can be analyzed conveniently by replacing the potential in the original Mathieu equation with a model one. Consequently, the function $\chi(\varphi)$ is described by

$$\left[-\frac{\partial^2}{\partial\varphi^2} + 2b^2 \sum_{n=0}^{M-1} \delta(\varphi - \varphi_n)\right]\chi = \varepsilon\chi, \tag{47}$$

where

$$b = N_0 L\omega_0/M, \quad \varepsilon = 2N_0 LE, \quad \varphi_n = 2\pi n/M.$$

Equation (47) retains all the principal features of the original problem, but it can be analyzed more simply. The spectrum of Eq. (44) is found by solving the transcendental equation

$$\cos\left(\frac{2\pi}{M}\left(m + \left\{\frac{\Phi}{\Phi_s}\right\}\right)\right) = \cos\frac{2\pi\varepsilon^{1/2}}{M} + \frac{b^2}{\varepsilon^{1/2}}\sin\frac{2\pi\varepsilon^{1/2}}{M}, \tag{48}$$

where $0 \leqslant m \leqslant M-1$.

The periodicity of the energy along the flux, with period Φ_s, and a dispersion law of the form (35) but with a different value of ε_0 in the tight-binding approximation ($b \to \infty$) follows from Eq. (48), but this is an artificial effect due to the assumptions made above.

4. FRACTIONALLY CHARGED SOLITONS AND AHARONOV-BOHM OSCILLATIONS

In the preceding section it is shown that temperature suppresses the oscillatory effects due to the macroscopic tunnel transitions. However, in the case of the system under discussion we can generally have an additional AB oscillation mechanism associated with the contribution of excited free carriers to the free energy.

Phase solitons ar charge carriers in a commensurate CDW. They have a low energy[14,15]

$$E_s = 8N_0\omega_0 c_0/M^2 \ll \Delta$$

and a fractional charge

$$q_f = \int dx j_0^{CDW} = \pm 2e/M$$

so that at low temperatures $T \ll \Delta_0$ they should dominate the oscillatory part of the free energy. Since the equilibrium density of soliton–antisoliton pairs increases with temperature, we can expect an anomalous temperature dependence of the quantum oscillations: their amplitude should increase with temperature. Finally, the period of the oscillations associated with fractionally charged solitons is of fundamental interest. In fact, in the naive approach the minimum period is $\Phi_f = 2\pi/q_f = M\Phi_0/2$, which is in conflict with the general conclusion that for $M > 2$, a system of integral charges (electrons) has only the fundamental period Φ_0 and its harmonics.

Our task is thus to calculate the free energy of solitons and antisolitons for a commensurate CDW having ring geometry, located in the field of an AB solenoid. In general, for an arbitrary ring and an arbitrary temperature T it is very difficult to solve this problem, but at low temperatures $T \ll E_s$ and in the case of sufficiently long rings $L \gg d$ ($d^{-1} = \omega_0/c_0$ is the characteristic size of a CDW soliton) the necessary expressions are easily obtained. In fact, for $T \ll E_s$, the density of thermally excited pairs is exponentially small and solitons in a given chain can be regarded as noninteracting, since the average distance between them is much greater than their characteristic dimensions. Here we can use the Coleman theorem[16] on the fermion–boson equivalence according to which the Lagrangian of free solitons in the sine–Gordon model is equivalent to the Dirac Lagrangian of zero-spin fermions ψ of mass $m_s = E_s/c_0^2$. As a result of "fermionization" the topological current of a CDW reduces to a standard electrodynamic fermion current $q_f\bar{\psi}\gamma_\mu\psi$ (see, for example, Refs. 15–17) and the Lagrangian of interest to us assumes the simple form ($\hbar = c_0 = 1$)

$$\mathscr{L}=\bar{\psi}[i\gamma_\mu(\partial_\mu-iq_fA_\mu)-E_s]\psi. \tag{49}$$

In a ring the fermion wave function ψ should satisfy the physical boundary conditions. The usual requirement of periodicity $\psi(t,0) = \psi(t,L)$ automatically leads to oscillations with an anomalous period Φ_f. We recall however that in terms of the scalar field φ (phase) one circuit round the ring corresponds to a change in the phase by 2π, which in turn is equivalent to the transfer of a charge $2e$ along a closed path. Therefore, a similar transfer of a fractional charge[3] does not represent an identity transformation and should be accompanied by an additional acquisition of the wave-function phase.

We can correctly formulate the boundary condition for the wave function of fractionally charged objects by noting that within the interval $\varphi\in(0,2\pi)$ there are M different vacuum states $\varphi_\varkappa^0 = (2\pi/M)\varkappa$ ($\varkappa = 0, 1, ..., M-1$) and M corresponding identical types of solitons (antisolitons) $\varphi_{s(\bar{s})}^{\varkappa}(x)$ joining neighboring vacuum states. The boundary condition for the fermion wave function of each soliton ("fermionization" makes it possible to consider solitons as point objects, which is exceptionally convenient in specific calculations) is

$$\psi_{(\varkappa)}(t,L)=\exp\left(i\frac{2\pi}{M}\varkappa\right)\psi_{(\varkappa)}(t,0),\quad \varkappa=0,1,\ldots,M-1, \tag{50}$$

since only an M-fold circuit of a charge $q_f = 2e/M$ along a closed contour returns the system to its initial state. In calculating the thermodynamic characteristics we have to sum over all M branches of the spectrum.

Using Eq. (50), we find for each branch of the fermion spectrum of a ring of length L

$$\begin{aligned}\varepsilon_n^{(\varkappa)}&=[(p_n^{(\varkappa)}-q_fA)^2+E_s^2]^{1/2},\\ p_n^{(\varkappa)}&=\frac{2\pi}{L}\left(\frac{\varkappa}{M}+n\right),\quad \varkappa=0,1,\ldots,M-1.\end{aligned} \tag{51}$$

The density of the free energy of a gas of noninteracting particles and antiparticles is

$$F=\frac{T}{L}\sum_{\varkappa=0}^{M-1}\sum_{\substack{\gamma=\pm1\\ n=-\infty}}^{\infty}\ln\left\{1+\exp\left[-\frac{\varepsilon_n^{(\varkappa)}(\gamma)}{T}\right]\right\}, \tag{52}$$

where $\gamma_\pm$ is the sign of the soliton charge.

The sum in Eq. (52) can be calculated using the Poisson summation expression, so that after simple transformations we find that the oscillatory part of the free energy is given by

$$\begin{aligned}F^{\rm osc}=&-\frac{8}{L^2}\sum_{\varkappa=0}^{M-1}\sum_{k=1}^{\infty}\frac{1}{k}\cos\left[\frac{2\pi}{M}k\left(\varkappa+\frac{\Phi}{\Phi_s}\right)\right]\\ &\times\int_0^\infty dyy\sin(2\pi ky)\left[y^2+\left(\frac{LE_s}{2\pi}\right)^2\right]^{-1/2}\\ &\times\left\{\exp\left(\frac{2\pi}{LT}\left[y^2+\left(\frac{LE_s}{2\pi}\right)^2\right]^{1/2}\right)+1\right\}^{-1}.\end{aligned} \tag{53}$$

Each of the M branches of the spectrum of fractionally charged solitons on a ring oscillates [as indicated by Eq. (53)] with an anomalous period $\Phi_f = M\Phi_s$ ($\Phi_s = \Phi_0/2$). However, these oscillations cannot be observed physically when they are separate. Any physically observable quantity uses a simultaneous contribution of all the branches of the spectrum and as a result of interference there remains only a period equal to Φ_s, as in the case of the instanton AB effect. In fact, in the expression for the oscillatory part of the free energy given by Eq. (53) we sum first over $\varkappa$. The result differs from zero only for harmonics k which are multiples of M and correspond exactly to oscillations with a period Φ_s:

$$\sum_{\varkappa=0}^{M-1}\cos\left[\frac{2\pi k}{M}\left(\varkappa+\frac{\Phi}{\Phi_s}\right)\right]=\delta_{k,nM}\cos\left(2\pi k\frac{\Phi}{\Phi_s}\right). \tag{54}$$

We now consider the case of low temperatures when $T\ll E_s$, which allows us to simplify the integrand in Eq. (53). Then, the oscillatory part of the free energy is

$$F^{\rm osc}\approx-\frac{4E_s}{\pi L}\sum_{n=1}^{\infty}\frac{K_1(LE_s[(nM)^2+(LT)^{-2}]^{1/2})}{[(nM)^2+(LT)^{-2}]^{1/2}}\cos\left(2\pi n\frac{\Phi}{\Phi_s}\right). \tag{55}$$

Since in a real situation we have $LE_s\gg1$, we can use an asymptotic expression for the modified Bessel function $K_1(x)$. We then obtain

$$\begin{aligned}F^{\rm osc}\approx&-\frac{2}{L}\left(\frac{2}{\pi}T_KE_s\right)^{1/2}\\ &\times\frac{\exp\{-ME_s[T_C^{-2}+(MT)^{-2}]^{1/2}\}}{[M^2+(T_C/T)^2]^{1/4}}\cos\left(2\pi\frac{\Phi}{\Phi_s}\right).\end{aligned} \tag{56}$$

According to Eq. (56), when temperature is increased the amplitude of the oscillations increases (and so does the density of free carriers) reaching a maximum value of the order of $(T_CE_s)^{1/2}\exp(-E_sM/T_C)$ for $T\gg MT_C$. This value is considerably less than the amplitude of the oscillations in the instanton AB effect described by Eqs. (33) and (34). However, at temperatures $T\gtrsim\omega_0$ (we recall that in the range of validity of the above expressions we have $T_C\ll\omega_0$) the main contribution to the temperature dependence of the oscillation amplitude is made specifically by the soliton AB effect. As expected, this high-temperature limit corresponds to an activation energy representing a complex of M phase solitons carrying an integral charge $2e$. We must stress once again, that in contrast to the temperature dependence of the oscillation amplitude given by Eq. (56), in the case of metals this dependence is just the opposite: the amplitude decreases as a function of temperature in accordance with the law $\exp(-T/T_m)$, with $T_M = \hbar v_F/L$ (Ref. 1). In the next section we shall show that this law of temperature suppression of the oscillations applies also to conductors with an incommensurate CDW.

5. INSTANTON AHARONOV–BOHM EFFECT IN AN INCOMMENSURATE CHARGE-DENSITY WAVE

The Lagrangian of an incommensurate CDW

$$\mathscr{L}_{eff}(\varphi)=\frac{N_0}{2}\left[\dot{\varphi}^2+c_0^2\varphi'^2+i\frac{2eA}{\pi N_0}\dot{\varphi}\right] \tag{57}$$

is quadratic in the field $\varphi(x, \tau)$ and the partition function for the phase degree of freedom can therefore be calculated exactly. As in Sec. 3, we shall consider classical vacuum–vacuum paths in imaginary time as well as small deviations from these paths. The partition function of such a system is factored into a partition function of phasons independent of the flux (the phasons are now the Goldstone excitations) and a cofactor Z_t which is due to the contribution of topologically nontrivial fluctuations.

The classical vacuum–vacuum paths satisfy the following cyclic boundary conditions

$$\varphi(\tau, 0)-\varphi(\tau, L)=2\pi n, \quad \varphi(\tau, x)-\varphi(\tau+\beta, x)=2\pi m \tag{58}$$

(n and m are integers), so that the partition function of interest to us is

$$Z_t=\sum_{m,n=-\infty}^{\infty} \exp(-S_{mn}), \tag{59}$$

where

$$S_{mn}=um^2+im\theta+wn^2, \quad \theta=2\pi\Phi/\Phi_s, \tag{60}$$

$$u=2\pi^2 LN_0/\beta, \quad w=2\pi^2\beta N_0 c_0^2/L. \tag{61}$$

The series in Eq. (59) can be summed exactly:

$$Z_t=\vartheta_3(0, q_w)\vartheta_3(v, q_u). \tag{62}$$

Here, $\vartheta_3(v,q)$ is a Jacobi function, $v=\theta/2\pi$, and $q_x=e^{-x}$. The free-energy correction oscillating with the flux is due to the contribution of large spatially homogeneous fluctuations which alter the phase by a multiple of 2π, and it follows from Eq. (62) that this correction is

$$F^{\text{osc}}=-\frac{1}{\beta}\ln\vartheta_3(v, q_u)=-\frac{1}{\beta}\ln\Big[1+2\sum_{m=1}^{\infty} q_u^{m^2}\cos(2\pi mv)\Big]. \tag{63}$$

For $u\gg 1$ (high temperatures), it follows from Eq. (63) that

$$F^{\text{osc}}_{(\beta)}\approx -2T\exp\Big(-\pi\frac{Tv_F}{T_C c_0}\Big)\cos\Big(2\pi\frac{\Phi}{\Phi_s}\Big). \tag{64}$$

The expression (64) follows directly, apart from a preexponential factor, from Eqs. (36), (39), and (41) if $M=1$. In fact, at high temperatures, $T\gg\omega_0$, a corrugated relief of the potential energy of a CDW ($\sim\omega_0^2\cos M\varphi$) becomes unimportant compared with the contribution made to the kinetic energy and we are then dealing with a Lagrangian of an incommensurate CDW. We note that an exponential fall of the oscillation amplitude with temperature is typical of metals.[1] An important feature of conductors with a CDW is the appearance of a superconducting flux quantum in the main oscillation period.

We can reach the limit of low temperatures in Eq. (63) by rewriting ϑ_3 using the imaginary Jacobi transformation[18]:

$$\vartheta_3(v\,|\,\tau)=(-i\tau)^{-1/2}\exp\Big(\frac{i\pi v^2}{\tau}\Big)\vartheta_3\Big(\frac{v}{\tau}\Big|-\frac{1}{\tau}\Big), \tag{65}$$

which in our case gives the expression

$$\vartheta_3\Big(\frac{\theta}{2\pi}, e^{-u}\Big)=\Big(-\frac{\pi}{\ln q}\Big)^{1/2}\exp\Big(\frac{\theta^2}{4\ln q}\Big)\vartheta_3\Big(i\frac{\theta}{2\pi q}, \exp\Big(\frac{\pi^2}{\ln q}\Big)\Big), \tag{66}$$

with $\ln q=-u=-\pi Tv_F/T_C c_0$. Using the asymptotic form for $T\to 0$, we then obtain

$$\vartheta_3\Big(\frac{\theta}{2\pi}, e^{-u}\Big)\approx\Big(\frac{\pi}{u}\Big)^{1/2}\exp\Big(-\frac{\theta^2}{4u}\Big). \tag{67}$$

It therefore follows that the low-temperature limit to the oscillatory free-energy correction is independent of temperature and is given by

$$F^{\text{osc}}_{(0)}\approx -T_C\frac{c_0}{v_F}\Big\{\frac{\Phi}{\Phi_s}\Big\}^2, \quad T_C=\frac{\hbar c_0}{L}. \tag{68}$$

According to Eq. (68), the oscillations of an incommensurate CDW "survive" even at absolute zero. Their period is equal to a superconducting flux quantum $\Phi_s=\Phi_0/2$ and the amplitude is governed by the Casimir "temperature" T_C representing size quantization of a CDW (a small factor $c_0/v_F\ll 1$ reflects the inertia of a collective degree of freedom, i.e., of a CDW, compared with one-electron excitation). It should be noted that in contrast to all the AB oscillation mechanisms considered above, the amplitude of the low-temperature oscillations of an incommensurate CDW, $T\ll T_C c_0/v_F$, does not contain an exponentially small factor. This feature is closely related to the scaling symmetry of the Lagrangian of Eq. (57) and, as shown above, it disappears if we allow for pinning of the commensurability. It is well known that in real systems a CDW is always pinned (see, for example, Ref. 6). The results given in Secs. 3 and 5 apply to phase excitations in an isolated chain. In the next section we shall allow for the influence of a three-dimensional interchain interaction on the instanton AB effect.

6. INFLUENCE OF THE INTERCHAIN INTERACTION ON THE INSTANTON AHARONOV–BOHM EFFECT

The interchain interaction Hamiltonian is (see, for example, Ref. 9)

$$H_{ij}=W\sum_{n,\Delta}[1-\cos(\varphi_n-\varphi_{n+\Delta})], \tag{69}$$

where n is the chain number and the index Δ labels the nearest neighbors. The influence of the term (69) on the instanton AB effect is easiest to study by considering the example of two interacting chains with incommensurate CDWs. Since we are interested in the coherent reaction of a CDW to a solenoid field, we shall assume that the phase is spatially homogeneous ($\partial_x\varphi=0$) and, for simplicity, we shall write down $L=N_0=1$. The Lagrangian of such a quantum-mechanical system is

$$\mathscr{L}=\frac{1}{2}\dot\varphi_1^2+\frac{1}{2}\dot\varphi_2^2-\frac{e}{\pi}A(\dot\varphi_1+\dot\varphi_2)-W[1-\cos(\varphi_1-\varphi_2)]$$
$$=\frac{1}{4}\dot\eta^2+\frac{1}{4}\dot\xi^2-\frac{e}{\pi}A\dot\xi-W(1-\cos\eta), \tag{70}$$

where $\varphi_{1,2}$ are the phases of a CDW for each of the chains; $\eta=\varphi_1-\varphi_2$, $\xi=\varphi_1+\varphi_2$. The Hamiltonian corresponding to Eq. (70) is

$$H=\hat{P}_\eta^2+\left(\hat{P}_\xi+\frac{e}{\pi}A\right)^2+W(1-\cos\eta),$$

$$\hat{P}_\eta=\frac{1}{i}\frac{\partial}{\partial\eta},\quad \hat{P}_\xi=\frac{1}{i}\frac{\partial}{\partial\xi}. \tag{71}$$

The wave function ψ in the Schrödinger equation has independent periods equal to 2π in terms of each of the variables φ_1 and φ_2. As we have seen already, oscillations with the period Φ_s are due to periodicity in ξ with period 2π. However, it follows from the periodicity in terms of $\varphi_{1,2}$ that the shift of ξ by 2π involves a shift of η by 2π, so that

$$\psi(\xi,\eta)=\psi(\xi+2\pi,\eta+2\pi)=\psi(\varphi_1+2\pi,\varphi_2). \tag{72}$$

In the plane of the two variables (ξ, η) the motion along the ξ axis occurs in a valley and along the η axis it necessarily passes through a maximum of the interaction potential (curve 1 in Fig. 2). Consequently, the amplitude of a harmonic with period Φ_s must contain the factor $\exp(-8W^{1/2})$. In the limit $W\to\infty$ the harmonic Φ_s disappears from the expression for the energy.

On the other hand, the amplitude of the harmonic $\Phi_s/2$ survives in the limit $W\to\infty$, since there is a path (curve 2 in Fig. 2),

$$\psi(\xi,\eta)=\psi(\xi+4\pi,\eta)=\psi(\varphi_1+2\pi,\varphi_2+2\pi), \tag{73}$$

which passes completely along a valley parallel to the axis of the variable ξ. The amplitude of this harmonic is independent of the intensity W of the interchain interaction.

It therefore follows that the role of the interchain interaction reduces to suppression of the fundamental harmonic which has the period Φ_s. In the limit of a strong interchain correlation a flux quantum splits up; the main period of the oscillations becomes equal to $\Phi_s/2$. Clearly, the amplitude of the $\Phi_s/2$ harmonic contains in the tunnel action the number of chains, since the action is an integral of the period. In this case, the integration range extends from 0 to 4π and not to 2π, as in the case of one chain. The physical interpretation of this result is quite obvious: in the limit $W\to\infty$ the phases of the chains become equalized and an instanton with a double charge and a double mass moves in the field of the flux.

These conclusions are readily generalized to the case of an arbitrary number of chains. If we have a system of N noninteracting chains ($W=0$), we find that the total partition function factors:

$$Z_N=Z_1^N, \tag{74}$$

where Z_1 is the partition function of one chain, and the final

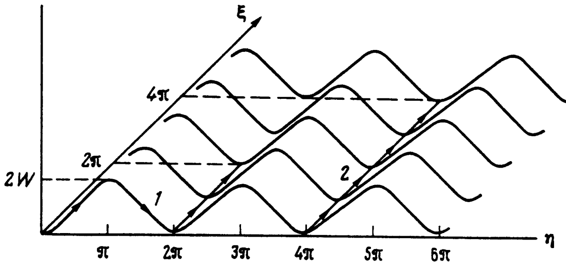

FIG. 2. Potential relief in the plane of the variables ξ and η. Here, 1 denotes the path corresponding to a harmonic with the period Φ_s and 2 corresponds to one with a period $\Phi_s/2$.

expressions for F^{osc} simply increase by N. In the presence of correlations there is only one path in the space of N variables corresponding to the period $2\pi N$ that can be expressed in terms of the combined coordinate

$$\Xi=\sum_{n=1}^{N}\varphi_n,$$

which does not intersect the potential barriers formed by the interchain interaction. A flux quantum corresponding to such a path is Φ_s/N. The amplitude of these oscillations contains the exponential factor $\exp(-NS_0)$. Consequently, the amplitudes of the oscillations with the periods $\Phi_s/(N-p)$ $(p=0, 1, 2, ..., N-1)$ contain the factors

$$F^{osc}_{N-p}\propto\exp[-S_0(N-p)-8W^{1/2}p], \tag{75}$$

corresponding to passage across p interchain barriers, and in the limit $W\to\infty$ this amplitude vanishes.

A real situation corresponds more closely to the case of correlated chains and a numerical increase in the argument of the tunnel exponential function by a factor of N can be compensated by selecting a small ring perimeter L. For example, in the case of parameters of the commensurate compound TaS_3 for $L\sim c_0/\omega_0\sim 10^3$ Å and a number of chains $N\sim 10^2$, the argument of the tunnel exponential function is of order 5 (Ref. 19).

CONCLUSIONS

The main result of the present investigation is the demonstration of the existence of a fundamentally new mechanism for AB oscillations encountered in insulators with a CDW, which differs from the usual AB effects discussed so far (for review see Refs. 20–22). The new effect is manifested by oscillations of the thermodynamic quantities as a function of the flux with the period $hc/2e$ corresponding to a superconducting quantum and it is simply a manifestation of the Fröhlich mechanism of superconductivity in systems with the CDW. Pinning of a CDW causes the AB effect to be absent in infinite systems, so that only systems of dimensions comparable with the coherence length can exhibit this effect. One should mention here Ref. 23, where attention is drawn to the existence of the AB effect in a one-dimensional superconductor which has no long-range order.

The AB effect in systems with a CDW is due to the tunneling of quantum states of an insulator ring as a whole and is a manifestation of the macroscopic quantum coherence. Its experimental detection would confirm an important (from the general theoretical point of view) conclusion that a quantum-mechanical description can be extended to macroscopic nonsuperconducting systems.

The AB effect in normal metals has been observed experimentally so far using a nonmonotonic dependence of the resistance of a ring on the magnetic flux,[21] but there is another possibility mentioned in Ref. 1, which is based on oscillations of the magnetic susceptibility. The magnetic moment of a ring is

$$\mu=-S\frac{\partial E}{\partial\Phi}, \tag{76}$$

where S is the area bounded by the ring. The part of the moment μ which oscillates with a period has the following amplitude at $T=0$:

$$\mu_{\rm osc}\sim S\frac{\hbar\omega_0}{\Phi_s}\left(\frac{S_0}{\hbar}\right)^{1/2}\exp\left(-\frac{S_0}{\hbar}\right). \qquad (77)$$

We shall now estimate the oscillation amplitude for a one-chain ring formed, for example, from TaS_3. The one-instanton action S_0 is governed [see Eq. (31)] by the perimeter L of the ring, by the phason velocity c_0, and by the phason soliton energy E_s. The value of E_s can be found by investigating the nonlinear component of the conductivity of a CDW, which is[6,7]

$$\sigma_{nl}\propto\exp\left(-\frac{\varkappa}{\mathscr{E}/\mathscr{E}_T-1}\right),\quad \varkappa=\frac{\mathscr{E}_0}{\mathscr{E}_T}. \qquad (78)$$

Here, $\mathscr{E}$ is a static electric field; $\mathscr{E}_T$ is the threshold field for the appearance of a nonlinear conductivity; $\mathscr{E}_0$ is the activation field. The experimental values of TaS_3 are $\mathscr{E}_T = 2.2$ V/cm and $\varkappa = 5$. According to Refs. 19 and 24, the value of $\varkappa$ determines the energy E_s of the phase solitons. It follows from Refs. 6 and 7 that $c_0 \sim 10^7$ cm/s and the characteristic length of phase inhomogeneities (soliton length) is 10^3–10^4 Å. Substitution of these parameters into the expression for $\varkappa$ gives the soliton energy $E_s \sim 1$ K. The same estimate follows from an analysis of the temperature dependence of the activation energy of the nonlinear conductivity of a CDW (Ref. 25). Therefore, we find that the argument of the exponential function in Eq. (77) is $S_0/\hbar \sim 10^4\ {\rm cm}^{-1}\cdot L$. The pinning energy of the commensurability is of order 10^{-2}–10^{-1} K. Consequently, in the case of rings of micron dimensions we have $\mu_{\rm osc} \sim 10^2 \mu_B$ (μ_B is the Bohr magneton). In principle, such moments can be determined using SQUIDs.[26] If we now consider a bulk sample consisting of many rings, we have to allow for imperfections of the atomic structure which in the simplest case may reduce to the appearance of a certain number (q) of chains which are not closed. Then, Eq. (75) should be modified by replacing N with $N - q$. An estimate of $\mu_{\rm osc}$ now has an additional factor of the type given by Eq. (75). In view of technological difficulties which would be encountered in the fabrication of such rings, this quantity is not known in advance and further theoretical and experimental investigations are desirable.

It is interesting to consider briefly some of the problems not resolved above. The most important of these is clearly the influence of dissipation on the instanton AB effect. A fairly strong dissipation (like high temperatures) undoubtedly destroys the quantum coherence and suppresses the AB oscillations. Under weak dissipation conditions a perturbation theory treatment of the effective interaction of instantons, induced by the dissipative nonlocal (in imaginary time) term in the Lagrangian of eq. (10), clearly just reduces to the renormalization of the oscillation amplitude. However, if a ring is subjected to the AB effect alternating in time $\Phi(t)$, the Josephson oscillations caused by the flux quantization[27] can have not only the canonical period $T_s = \Phi_s/\dot{\Phi}$, but also a period $T_f = \Phi_f/\dot{\Phi}$ which is M times longer and which is due to slip of a fractionally charged ($q_f = 2e/M$) instanton if the inequality $\omega\tau \gg 1$ is obeyed; here τ is the inelastic scattering time (Fig. 3).

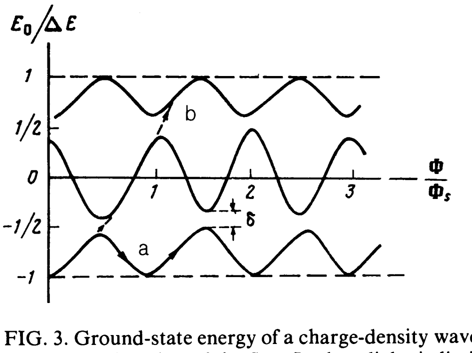

FIG. 3. Ground-state energy of a charge-density wave in the case $M = 3$, plotted as a function of the flux. In the adiabatic limit the system moves along the curve a, corresponding to the energy minimum. This curve describes thermodynamic ($\omega\to 0$) oscillations with the period Φ_s. For $\omega \gg 1/\tau$ and $\omega \gg \delta$, instanton slip is possible and the system moves along a curve of constant m with a period equal to a "fractional" (representing a fraction of the charge $2e/M$) quantum of the flux $M\Phi_s$ (curve b).

The next (in importance) topic ignored above is the influence of impurities on the present effect. Since in the instanton AB effect the tunneling is macroscopic, impurities (in contrast to temperature or dissipation) cannot play a decisive role in the destruction of the quantum coherence. In a systematic approach they should be allowed for in the microscopic (electron–phonon) Hamiltonian so that the effective long-wavelength Lagrangian of the phase given by Eq. (8) may contain only the correlation characteristics of the impurity field. This problem was solved in the case of weak impurity pinning for a commensurate CDW in Ref. 28, where it was shown that the influence of impurities is important only in a quantum description of a CDW. In particular, in the case of the CDW Lagrangian of Eq. (8) there are additional terms induced by forward-scattering impurities. In our problem these terms simply modify the one-instanton action slightly. It should be noted that the impurities suppressing the order parameter reduce the energy of topological solitons[28,29] and, therefore, should increase the oscillation amplitude in the soliton AB effect. This anomalous behavior (in the one-particle AB effect the role of impurities is just the opposite) is explained by the fact that CDW solitons are extended nonlinear excitations of the order parameter and the influence of weak impurities on their properties appears primarily because of renormalization of the parameters of the effective phase Lagrangian. Naturally, these preliminary conclusions must be checked.

Finally, there is a very interesting problem of the role of strong impurity pinning when the ground state of a CDW may be greatly modified (for example, a vacuum state of a CDW may become inhomogeneous).

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[1)] The first experimental observations of the AB oscillations with period hc/e were reported in Ref. 3; those with the period $hc/2e$ were reported in Ref. 4.

[2)] For $L \lesssim (\omega_0/c_0)^{-1}$, an important point is the inclusion of the quantum fluctuations of the phase, which result in modification of the semiclassical Lagrangian of Eq. (8).

[3)] This applies naturally not to an elementary fractional charge, but to a fractional charge that appears because of the polarization of the vacuum state of integral elementary charges by a topologically nontrivial external field.

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