Macroscopic quantum tunneling of a three-dimensional charge-density wave in an above-threshold electric field

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A theory of macroscopic quantum tunneling of a three-dimensional commensurate charge-density wave in an above-threshold electric field $E > E_T$ is developed. The size and shape of the tunneling seed are determined and the tunneling action is calculated. The numerical values of the TaS_3 seed parameters are estimated. The seed contains macroscopic (on the order of several hundred conducting chains) segments of plane soliton–antisoliton walls that produce the threshold tunnel-creation threshold field. The contribution of the plane walls to the action is found to be decisive.

A number of quasi-one-dimensional conductors, such as tri- and tetrachalcogenides of transition metals ($NbSe_3$, TaS_3, $(TaSe_4)_2I$, $(NbSe_4)_{3.33}I$, NbS_3 and others) or bronzes (e.g., $K_{0.3}MoO_3$, $Rb_{0.3}MoO_3$) are in a dielectric Peierls state at temperatures lower on the average than 10^2 K (see the reviews in Refs. 1 and 2), i.e., they are Peierls dielectrics (PD). The order parameter of a PD is a complex quantity $\Delta \exp(i\varphi)$. Its modulus Δ determines the gap in the single-electron spectrum and its value is about several hundred degrees for all the above compounds. The phase φ describes the translational degree of freedom of the Peierls superstructure

$$x_n = na + u(n)\cos(2k_F na + \varphi(n)) \qquad (1)$$

(a is the lattice constant, k_F is the Fermi momentum, and $u \sim \Delta$). The derivatives of the phase determine the charge density and the current that are due to local fluctuations of the chemical potential if the electron "basement" (the valence band) is completely filled with electrons:

$$\delta\rho = \frac{e}{\pi}\frac{\partial\varphi}{\partial x}, \quad j = -\frac{e}{\pi}\frac{\partial\varphi}{\partial t} \qquad (2)$$

and determine the response (1) of the charge-density wave (CDW).

Typical energies connected with the phase degree of freedom in PD are smaller by several orders than the single-electron energies ($\sim\Delta$). It is therefore the CDW motion that causes the PD current-voltage characteristics (IVC) observed in electric fields E to be small compared with Δ at temperatures when the number of normal carriers is exponentially small [$\sim\exp(-\Delta/T)$]. The main distinctive feature of the IVC of PD is the existence of threshold nonlinearities (a distinction is made between the low-temperature and high-temperature thresholds[3]). The static threshold fields E_T at which nonlinear responses are produced are weak, from 0.01 (V/cm in the low-temperature phase of $NbSe_3$ to 20 V/cm in NbS_3.

The nonlinear IVC of CDW are described at present by two theoretical approaches—the classical model of the CDW and the quantum tunnel model (Refs. 1–4). In the classical scheme the phase φ_c is regarded as a homogeneous dynamic variable that obeys one-dimensional equations of the Josephson type. The analog of the Josephson energy is the so-called commensurability energy $\propto \cos M\varphi$ (Ref. 5), where M is an integer ($M > 2$), $M = 4$ for TaS_3 and $NbSe_3$. The presence of commensurability energy ensures an $E_T^{(c)}$ threshold above which $\overline{\partial\varphi_c/\partial t} \neq 0$ (the overbar denotes time averaging). The IVC calculated in the classical model describes fairly well the high-temperature region of the nonlinear phenomena.[6] At the same time, the classical model cannot explain the IVC observed above the low-temperature threshold. Namely, the empirically determined field dependence of the static conductivity is

$$\sigma(E) = \sigma_0 + (1 - E_T/E)\sigma_1 \exp[-E_0/(E - E_T)]\theta(E - E_T), \qquad (3)$$

where σ_0 is the ohmic component and θ is the Heaviside step function.

Disregarding the presence of a threshold in the exponential, the second term of (3) has the typical tunneling form. The values of the activation field $E_0 \ll \Delta^2/e\hbar v_F$ (v_F is the Fermi energy), however, is weak so that Zener production of electrons cannot explain the relation (3). To explain (3), a special quantum model was proposed, in which the conductivity is due to tunneling creation, independently on each PD chain, of special nonlinear carriers, viz., phase solitons and antisoliton pairs similar to the electron–hole pairs in Zener breakdown of a dielectric. In fact, the equation for a one-dimensional commensurate CDW is a sine-Gordon equation having soliton solutions. The energy of the CDW soliton is determined by the commensurability potential, which is much smaller than Δ. It was this which made it possible in principle to account for the smallness of E_0. Analysis of the experimental data, however, shows that, first, the E_0 calculated in the independent-soliton approximation is smaller by one or two orders than the observed one and, second, no threshold field E_T appears in such a theory. These difficulties are eliminated by taking into account interactions between the electron chains, when the solitons turn out to be in the confinement phase.[7,8] The field produces in this case soliton complexes that contain many chains, E_0 increases to observable values, and the onset of E_T has a threshold due to the Coulomb interaction of the soliton–antisoliton walls. The idea of the influence of confinement on soliton production by an electric field was proposed in Ref. 7, partially confirmed in Ref. 8, and independently stated in Ref. 4. In contrast to Refs. 7 and 8, however, no account was taken in Ref. 4 of the Coulomb interaction of the solitons and antisolitons, and the role of the confinement was reduced only to a renormalization of E_0.

The statement in Refs. 7 and 8 did not prove the hypothesis that the tunneling-seed soliton–antisoliton walls are

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plane. This assumption is proved in the present paper, the main purpose of which is a determination, in the microscopic CDW theory, of the form of the tunneling seed.

We shall show that the tunneling seed is cigar-shaped. It is elongated in the one-dimensionality direction. The longitudinal size of the seed is inversely proportional to the difference $E - E_T$, while the transverse dimension is approximately one-tenth the width d of the soliton wall. Using the experimental parameters of the problem, we calculate the soliton energy (it turns out to be of the order of a fraction of one degree) and the number N_k of chains in the seed (of order 10^2–10^3). The width d of the soliton wall is about several thousand lattice constants. The ends of the "cigar" contain macroscopic flat sections that produce the soliton–antisoliton electrostatic confinement field E_T. The contribution made to the action by the plane sections is predominant and takes the form (3) on satisfaction of the conditions of quasi-one-dimensionality and of the standard "thin-wall" approximation (for the longitudinal direction). The latter approximation is known from the theory of macroscopic tunneling (see, e.g., Ref. 9) and is equivalent to creation of free soliton–antisoliton pairs at a small excess above threshold, i.e., at $1 \gg (E/E_T - 1) > 0$. The necessary criteria are obtained for the parameters of the substances and for the field strength.

1. EFFECTIVE LAGRANGIAN OF TUNNELING SEED

Consider the generating CDW functional (see the Appendix)

$$\mathscr{F}_{CDW} = -i \ln \int D\varphi \exp\left[i \int d\mathbf{r}\, dt \mathscr{L}(\varphi) \right], \tag{4}$$

where $\mathscr{L}(\varphi)$ equals according to Ref. 8 ($\hbar = 1, c = 1$)

$$\mathscr{L}(\varphi) = \frac{1}{2} N_0 n_f \left\{ \dot{\varphi}^2 - c_\parallel^2 \left(\frac{\partial \varphi}{\partial x}\right)^2 - c_\perp^2 (\nabla_\perp \varphi)^2 + \frac{2\omega_0^2}{M^2}(\cos M\varphi - 1) - \omega_\varphi^2 \varphi^2 \right\} - \frac{e}{\pi} n_f A \dot{\varphi} + \frac{e^2 n_f^2}{2\pi^2 \varepsilon_\parallel^{3/2}} \int d\mathbf{r}' (\nabla_\perp \varphi)(\nabla_\perp' \varphi) \times \left[\frac{(x-x')^2}{\varepsilon_\parallel} + \frac{|\mathbf{r}_\perp - \mathbf{r}_\perp'|^2}{\varepsilon_\perp} \right]^{-1/2}. \tag{5}$$

Here $N_0 = 2\Delta^2/\pi\overline{\omega}^2 v_F$, $\omega_\varphi^2 = 2\overline{\omega}^2 e^2 n_j \xi_0/\pi\varepsilon_\parallel \Delta$, $\xi_0 = v_F/\Delta$, $\omega_0 = \mu M \overline{\omega}$, $c_{\parallel,\perp} = (\overline{\omega}/2\Delta) v_{F,\perp}$, $v_\perp \ll v_F$ is determined by the effective transverse dispersion of the electrons and phonons, $\overline{\omega}$ is the Debye frequency, $\mu \sim (\Delta/\varepsilon_F)^{M/2-1} \ll 1$, $A = -Et$, E is the external electric field, n_f is the two-dimensional density of the dielectric chains, and $\hat{\varepsilon}_{\alpha\beta}$ is the dielectric tensor.

Contributions to the integral can be made by classical trajectories φ^c in both real and imaginary time (instantons). The CDW current

$$j = \frac{\delta \mathscr{F}_{CDW}}{\delta A} = -\frac{e}{\pi} n_f \sum_{\{i\}} \mathrm{Re} \left\langle \frac{\partial \hat{\varphi}_i}{\partial t} \right\rangle \tag{6}$$

is the sum of the contributions of the "partial" currents corresponding to each trajectory φ_i^c after averaging over the quantum fluctuations $\delta\varphi_i$ ($\hat{\varphi}_i = \varphi_i^c + \delta\varphi_i$). For the real-time trajectories $\varphi_R(x,t)$ we can neglect the contribution of the quantum fluctuations, and the classical part of the CDW current takes the standard form [cf. Eq. (2)]

$$j_c = -(e/\pi) n_f \partial\varphi_R/\partial t. \tag{7}$$

For Euclidean trajectories $\varphi_I(x,it)$ a nonzero current (6) is obtained only after averaging over the quantum fluctuations, when the effective action acquires an imaginary part.[10] The quantum part of the CDW current is thus

$$j_q = -(e/\pi) n_f \mathrm{Re} \langle \partial\hat{\varphi}_I/\partial t \rangle \propto \exp(-S_{eff}). \tag{8}$$

Here S_{eff} is the tunneling action calculated from the Lagrangian (5) on a Euclidean (instanton) classical trajectory. This is in fact the current considered in the quantum model of the CDW conductivity.[7,8,11] The analysis shows that the quantum and classical components of the CDW conductivity are additive.

A quasi-one-dimensionality criterion $\alpha^2 = c_\perp^2 \varepsilon_\parallel / c_\parallel^2 \varepsilon_\perp \gg 1$ was established in Ref. 8 for the CDW Lagrangian. When the condition $\alpha \gg 1$ is met the zeroth approximation of the CDW equation of motion is $\nabla_\perp \varphi = 0$ and the problem becomes effectively one-dimensional.

The density of the potential energy $U\{\varphi\}$ of the Lagrangian (5), which is a nonlocal functional of the phase

$$U\{\varphi\} = N_0 n_f \left\{ \frac{1}{2} c_\parallel^2 \left(\frac{\partial\varphi}{\partial x}\right)^2 + \frac{1}{2} c_\perp^2 (\nabla_\perp \varphi)^2 + \frac{\omega_0^2}{M^2}(1 - \cos M\varphi) + \omega_\varphi^2 \mathscr{E} \varphi \right\} + \frac{e^2 n_f^2}{2\pi\varepsilon_\perp \varepsilon_\parallel^{1/2}} \int d\mathbf{r}' \left(\frac{\partial\varphi}{\partial x}\right)\left(\frac{\partial\varphi}{\partial x'}\right) \left[\frac{(x-x')^2}{\varepsilon_\parallel} + \frac{|\mathbf{r}_\perp - \mathbf{r}_\perp'|^2}{\varepsilon_\perp} \right]^{-1/2}, \tag{9}$$

where $\mathscr{E} = E/\widetilde{E}$, $\widetilde{E} = en_f/\pi\varepsilon_\parallel$, has for $\alpha \gg 1$ the simple local limit[7]

$$U\{\varphi\} = N_0 n_f \{ c_\parallel^2 (\partial\varphi/\partial x)^2/2 + (\omega_0^2/M^2)(1 - \cos M\varphi) + \omega_\varphi^2 (\varphi + \mathscr{E})^2/2 \} \tag{10}$$

It is easy to change from (9) to (10) by using an identity based on the Poisson equation:

$$\varepsilon_\parallel \int d\mathbf{r}\, d\mathbf{r}' \frac{\partial\varphi}{\partial x} \frac{\partial\varphi}{\partial x'} \left[\frac{(x-x')^2}{\varepsilon_\parallel} + \frac{|\mathbf{r}_\perp - \mathbf{r}_\perp'|^2}{\varepsilon_\perp} \right]^{1/2} = 4\pi\varepsilon_\parallel^{1/2} \varepsilon_\perp \times \int d\mathbf{r}\, \varphi^2 - \varepsilon_\perp \int d\mathbf{r}\, d\mathbf{r}' (\nabla_\perp \varphi)(\nabla_\perp' \varphi) \times \left[\frac{(x-x')^2}{\varepsilon_\parallel} + \frac{|\mathbf{r}_\perp - \mathbf{r}_\perp'|^2}{\varepsilon_\perp} \right]^{-1/2}, \tag{11}$$

where φ satisfies the condition $\varphi(|\mathbf{r}| \to \infty) = 0$.

It is easily seen that the minimum of (10) is realized for the $\varphi = 0$ solution when $E < E_T = 4\pi e n_f / M\varepsilon_\parallel$ and for $\varphi = -2\pi/M$ when $E > E_T$. In conjunction with the boundary condition $\varphi(|\mathbf{r}| \to \infty) = 0$ this means that fields $E > E_T$ favor energywise the appearance of large phase fluctuations in which $\varphi = -2\pi/M$ and the total field is $E_{\text{tot}} = E - 2E_T$. The minimum size $2x_c$ of the fluctuations is determined from the energy-balance condition: the gain in the bulk energy of the field and the loss in the surface energy of the phase-separation boundary

$$2x_c (\varepsilon_\parallel / 8\pi n_f) [E^2 - (E - 2E_T)^2] = 2E_s, \tag{12}$$

where E_s is the domain-wall energy. The longitudinal critical dimension of the seed is therefore

$$2x_c=\frac{2E_s}{(2e/M)(E-E_T)}, \tag{13}$$

where $2en_f/M$ is the density of the topological charge of the wall. At zero temperature such fluctuations are created by a tunnel mechanism, while the domain walls carry the charge.

It is very important to note that a transition from (9) to (10), using (11) under the condition $|\nabla_\perp\varphi|\ll\alpha^{-1}$, is valid strictly speaking only for an infinite distribution of $\varphi(\mathbf{r})$. Actually Eq. (10) can be simply obtained from (9) at constant $\varphi(\mathbf{r}_\perp)$ by simple integration with respect to $\mathbf{r}'_\perp$ between infinite limits. For $\varphi(\mathbf{r}_\perp)$ that is bounded in space it is necessary to take into account edge effects, where the derivative $\partial\varphi/\partial\mathbf{r}_\perp$ is in general not small. This circumstance is important for the analysis of the tunneling-seed structure.

To take into account the tunneling exponential (8) we must know solutions having finite action in imaginary time τ and with asymptotes $\varphi(|x|\to\infty)=0$ and $\varphi(x\approx 0)=\to 2\pi/M$. For $\omega_\varphi\ll\omega_0$ these solutions of the one-dimensional CDW are the soliton–antisoliton pair of the sine-Gordon equation (see, e.g., Ref. 10)

$$\varphi_{s\bar{s}}=-\frac{4}{M}\left\{\operatorname{arctg}\exp\left[\frac{x+x_0(\tau)}{d(1+\dot{x}_0^2/c_\parallel^2)^{1/2}}\right]-\operatorname{arctg}\exp\left[\frac{x-x_0(\tau)}{d(1+\dot{x}_0^2/c_\parallel^2)^{1/2}}\right]\right\}, \tag{14}$$

$d=c_\parallel/\omega_0\sim\xi_0\mu^{-1/2}$, and $2x_0$ is the longitudinal dimension of the $s\bar{s}$ pair. Since the solution (14) is independent of $\mathbf{r}_\perp$, $\varphi_{s\bar{s}}$ describes not a single soliton–antisoliton pair, but an $s\bar{s}$ wall passing through the entire crystal in transverse direction. It is clear, however, that the action calculated on the trajectory (14) is infinite.

A finite action imposes on the tunneling trajectory the additional requirement that the transverse spatial dimension be finite. To reconcile (14) with this condition we assume for the structure of the tunneling seed that

$$x_0=x_0(\tau,\rho),\ 0\leqslant\rho\leqslant\rho_{max}=\rho^*,\ x_0(\rho^*)=0. \tag{15}$$

The shape of the seed is assumed for simplicity to be axisymmetric in the transverse dimension (ρ is the transverse radius).

If $x_0\gg d$, the use of a soliton–antisoliton noninteracting pair as the tunneling seed is justified, for in this case the soliton interaction is exponentially small. In the region $x_0\lesssim d$ the tunnel trajectory can be approximately described by a small-amplitude bound $s\bar{s}$ state (see, e.g., Ref. 10)

$$\varphi_{s\bar{s}}\approx-\frac{4}{M}\frac{x_0}{d}\operatorname{ch}^{-1}\frac{x}{d(1+\dot{x}_0^2/c_\parallel^2)^{1/2}}. \tag{16}$$

Since appreciable transverse gradients appear in the region $\rho\approx\rho^*$, the structure of the seed (16) is generally speaking not obvious beforehand. We show below, however, that even for large transverse gradients the form of $\varphi_{s\bar{s}}$ is determined from the solution of a one-dimensional sine-Gordon equation.

It can be shown that the boundary conditions

$$\varphi(|\mathbf{r}|\to\infty)=0,\ \varphi(|\mathbf{r}|<r_0)=-2\pi/M$$

and the requirement that the action be finite are compatible only with a positive curvature of the seed surface ($\partial x_0/\partial\rho<0$).

The electric field inside the seed is obtained as a solution of a Poisson equation with a charge density given by (2) and (14). It is easily seen that when $\varphi(\mathbf{r}_\perp)=\text{const}$, we have $E_\perp=0$ and the longitudinal electric field is equal to the value of the field in a parallel-plate capacitor with charge density $2|e|n_f/M$ on the electrodes. Assume now that $\varphi(\mathbf{r})$ is piecewise constant, $\varphi(\mathbf{r})=\varphi(x)\theta(\rho_0-\rho)$. For the distances between the charges that satisfy the condition $d\ll x_0\ll\rho_0(\varepsilon_\parallel/\varepsilon_\perp)^{1/2}$, in the region $\rho<\rho_0$, we have

$$E_x=-\frac{16en_f}{M\varepsilon_\parallel}\operatorname{arctg}\left(\frac{\rho_0-\rho}{x\varepsilon_\perp^{1/2}/\varepsilon_\parallel^{1/2}}\right) \tag{17}$$

(the condition $d\ll x_0$ is necessary to form opposite charges). At $\rho\ll\rho_0$ this expression tends to $(-8en_f\pi/M\varepsilon_\parallel)$. For $x_0\gg\rho_0(\varepsilon_\parallel/\varepsilon_\perp)^{1/2}$ the field of the plane section goes over into the field of a point charge and ceases to be effectively one-dimensional. These estimates are necessary for the understanding of the important role of the transverse gradients $|\partial x_0/\partial\rho|\ll 1$ (called the quasi-one-dimensionality condition) in our calculation. Namely, if $\alpha\gg 1$ the edge effects (the finite size of the plane section of the surface) are negligibly small in the region $d\ll x_0\ll\rho_0(\varepsilon_\parallel/\varepsilon_\perp)^{1/2}$. It is only in this region that a Coulomb potential ensures soliton confinement.

Using now (14) and (16) we obtain the phase effective Lagrangian that depends only on the instantaneous dimension $x_0(\tau,\rho)$ of the tunneling seed. We substitute (14) in the Lagrange function and integrate with respect to x and x', i.e., we change over to the effective Lagrangian from the collective degree of freedom x_0. In the region $x_0\gg d$ the effective Lagrangian is

$$l_{eff}(\dot{x}_0,x_0)=n_f\left\{-2E_s\left(1+\frac{\dot{x}_0^2}{c_\parallel^2}\right)^{1/2}+e^*x_0(E-E_T)-E_s\left(\frac{c_\perp}{c_\parallel}\right)^2\left(\frac{\partial x_0}{\partial\rho}\right)^2\right\}+\frac{\Gamma}{2}\int dx\,dx'\,f(x)f(x')\times\int d\rho'\rho'\left(\frac{\partial x_0}{\partial\rho}\right)\left(\frac{\partial x_0}{\partial\rho'}\right)g(\rho,\rho')\left[\frac{\varepsilon_\perp}{\varepsilon_\parallel}(x-x')^2+(\rho-\rho')^2\right]^{-1/2}, \tag{18}$$

$$g(\rho,\rho')=4\left(1+\frac{2}{k^2}\right)(1+k^2)^{-1/2}F\left(\frac{\pi}{2},\frac{k}{(1+k^2)^{1/2}}\right)-8\frac{(1+k^2)^{1/2}}{k^2}E\left(\frac{\pi}{2},\frac{k}{(1+k^2)^{1/2}}\right), \tag{19}$$

$$k^2=4\rho\rho'[\varepsilon_\perp/\varepsilon_\parallel(x-x')^2+(\rho-\rho')^2]^{-1}, \tag{20}$$

F and E are elliptic integrals,

$$g(\rho,\rho')\approx\begin{cases}2\pi, & k\ll 1,\\ (4/k)\ln 4k, & k\gg 1,\end{cases}$$
$$f(x)=\operatorname{ch}^{-1}[(x-x_0)/d]+\operatorname{ch}^{-1}[(x+x_0)/d], \tag{21}$$
$$\Gamma=2(4/M)^2\varepsilon_\perp^{1/2}n_f^2e^2/\varepsilon_\parallel^{3/2},$$

$e^*=2e/M$ is the fractional charge of the phase soliton, $E_s=8N_0\omega_0c_\parallel/M^2$ is its energy [cf. Eq. (13)], and $E_T=4\pi en_f/M\varepsilon_\parallel$.

In the region $x_0\lesssim d$, using (16), we get

$$l_{eff}(\dot{x}_0, x_0) = n_f\left\{-2E_s\left(\frac{\dot{x}_0}{c_\parallel}\right)^2\left(1+\frac{\dot{x}_0^2}{c_\parallel^2}\right)^{-1/2} - \frac{8}{3}E_s\left(\frac{x_0}{d}\right)^2 - E_s\left(\frac{c_\perp}{c_\parallel}\right)^2\left(\frac{\partial x_0}{\partial\rho}\right)^2 + 2e^*Ex_0 - \Omega_\varphi^2\left(\frac{x_0}{d}\right)^2\right\} + \Gamma\int d\rho'\left(\frac{\rho'}{\rho}\right)^{1/2}\frac{\partial x_0}{\partial\rho}\frac{\partial x_0}{\partial\rho'}G(\rho,\rho'), \quad (22)$$

where

$$\Omega_\varphi^2 = 128e^2n_fd/\pi^2M^2\varepsilon_\parallel,$$

$$G(\rho,\rho') = \frac{1}{2}\int_{-\infty}^{\infty}\frac{dx\,dx'}{\operatorname{ch}x\operatorname{ch}x'}\ln\left\{\frac{8(\rho\rho')^{1/2}}{[d^2(\varepsilon_\perp/\varepsilon_\parallel)(x-x')^2+(\rho-\rho')^2]^{1/2}}\right\}. \quad (23)$$

The Lagrangians (18) and (22) are the starting points for the calculation of the tunneling action.

2. CRITICAL DIMENSIONS OF SEED. CALCULATION OF THE TUNNELING ACTION

An exact solution of the tunneling problem implies determination of the instanton trajectory $x_0 = x_0\{\rho(\tau)\}$, but in the trial-function method which we are in fact using it suffices to choose a reasonable coordinate dependence $x_0(\rho)$ on the surface of the tunneling seed and to reduce the quantum-field problem to the quantum-mechanics problem for one dynamic variable $x_0(\tau)$. Decisive for the choice of $x_0(\rho)$ are the symmetry requirements. In our case, the strong anisotropy (quasi-one-dimensionality) and the small excess of the field above threshold (the approximation of thin walls along the field direction: $d \ll x_0$, Ref. 9) stipulate a cigar-shaped seed, with longitudinal dimensions appreciably larger than the transverse ones. This is precisely the form of the real (energywise favored) seed of the new phase (see below), so that it is natural to assume that the shape of the surface remains constant on the entire tunnel trajectory and is determined by the equation for the boundary of the seed on the mass shell[1)] ($\dot{x}_0 = 0$)

$$\mathscr{H}\{\dot{x}_0=0;\ x_0;\ \partial x_0/\partial\rho\}=0, \quad (24)$$

where $\mathscr{H}$ is the Hamiltonian constructed with the effective Lagrangians.

The foregoing assumption, of course, is certainly not satisfied at the very start of the tunneling in the interval $\tau < \tau_0$, when $x_0(\tau) \lesssim \rho^*$ (ρ^* is the maximum transverse dimension of the seed). It will be shown below that $\rho^* < d$, so that the interval τ_0 is wholly contained in the interval in which soliton walls are formed in the longitudinal direction, and makes a negligibly small contribution to the action when the threshold is only slightly exceeded.

Our main task is thus to solve the equation (24) for the surface of the critical seed. Unfortunately, there is no exact analytic solution for this equation, and we shall use perturbation theory.

In the region $x_0 \gg d$ the condition $\alpha \ll 1$ imposes, as a zeroth approximation of (24), for the one-dimensional problem the limiting points $x_0 = \pm x_c$ (13), while the transverse gradients are determined from the next-order approximation equation:

$$\frac{1}{2}\left(\frac{c_\perp}{c_\parallel}\right)^2\left(\frac{\partial x_0}{\partial\rho}\right)^2 - \frac{\Gamma}{4E_s}\int d\rho'\rho'\frac{\partial x_0}{\partial\rho}\frac{\partial x_0}{\partial\rho'}\int dx\,dx'g(\rho,\rho') \times f(x)f(x')\left[\frac{\varepsilon_\perp}{\varepsilon_\parallel}(x-x')^2+(\rho-\rho')^2\right]^{-1/2} = \frac{x_0-x_c}{x_c}. \quad (25)$$

If the $|\partial x_0/\partial\rho|$ are small in the finite region $\rho < \rho_T$, this region comprises flat walls and the one-dimensional approximation is valid.

It is clear, however, that as $\rho \to \rho^*$ the one-dimensional approximation is not valid and the perturbation theory must be based on the inverse parameter, assuming the contribution of the gradients to the energy to be decisive. We can thus determine the maximum transverse dimension ρ^* of the seed (at $x_0 = 0$). For the Lagrangian (22) Eq. (24) reduces to vanishing of a quadratic form of large transverse gradients. Denoting $\partial x_0/\partial\rho = p(\rho-\rho^*)$ and putting $\rho = \rho^*$ we obtain for the function p the equation

$$p(0) = \frac{2}{3}\frac{\rho^*}{\rho_0}p(0)G(\rho^*,\rho^*) - \frac{2}{3}\frac{1}{\rho_0(\rho^*)^{1/2}}\int_0^{\rho^*}d\rho'\rho'^{3/2}\frac{\partial}{\partial\rho'}[p(\rho'-\rho^*)G(\rho^*,\rho')]. \quad (26)$$

This equation has in the region $\rho^* - \rho \ll d(\varepsilon_\perp/\varepsilon_\parallel)^{1/2}$ the simple solution

$$\partial x_0/\partial\rho = \text{const} = -b, \quad b>0, \quad x_0 = b(\rho^*-\rho). \quad (27)$$

Equation (26) yields immediately the relation we need for the maximum transverse dimension:

$$\rho^*\tilde{G}(\rho^*,\rho^*) = {}^3/_2\rho_0, \quad (28)$$

where $\rho_0 = E_s(c_\perp/c_\parallel)^2n_f/\Gamma$, and

$$\tilde{G}(\rho^*,\rho^*) = \frac{\pi^2}{2}\ln\left[\frac{8\rho^*}{d(\varepsilon_\perp/\varepsilon_\parallel)^{1/2}}\right] - 2\int_0^\infty dy\frac{y\ln y}{\operatorname{sh}y} - \frac{3\pi^2}{8} = \frac{\pi^2}{2}\ln\left(\frac{3{,}8\rho^*\gamma}{d(\varepsilon_\perp/\varepsilon_\parallel)^{1/2}}\right), \quad (29)$$

$$\gamma = \exp[-{}^1/_3\ln 2 + (C-1) - 6\zeta'(2)/\pi^2] \approx 0.905, \quad (30)$$

C is the Euler constant and $\zeta(2)$ is the Riemann function.

We solve now Eq. (25). We introduce the function

$$\lambda = (c_\perp/c_\parallel)[2x_c(x_c-x_0)]^{1/2} \quad (31)$$

so that

$$\frac{\partial x_0}{\partial\rho} = -\frac{c_\parallel}{c_\perp}\left(2\frac{x_c-x_0}{x_c}\right)^{1/2}\frac{\partial\lambda}{\partial\rho}, \quad (32)$$

and obtain for λ the equation

$$\left(\frac{\partial\lambda}{\partial\rho}\right)^2 - \frac{1}{\rho^{(0)}}\int\left(\frac{\rho'}{\rho}\right)^{1/2}d\rho'\frac{\partial\lambda}{\partial\rho}\frac{\partial\lambda}{\partial\rho'}\int\frac{dx\,dx'}{\operatorname{ch}x\operatorname{ch}x'} \times \ln\frac{8(\rho\rho')^{1/2}}{[d^2(\varepsilon_\perp/\varepsilon_\parallel)(x-x')^2+(\rho-\rho')^2]^{1/2}} = -1, \quad (33)$$

where $\rho^{(0)} = \frac{1}{2}\rho_0(c_\parallel/c_\perp)^2$. For $\rho \to 0$ the solution of (33) is

$$\frac{\partial\lambda}{\partial\rho} = B\frac{(\rho/\rho^{(0)})^{1/2}}{\ln(\rho/\rho^{(0)})^{1/2}}, \quad (34)$$

and the constant B is determined from the relation

$$2\pi^2 B^2 \int_0^{\rho^T/\rho(0)} dy \frac{y}{\ln y} = 1. \quad (35)$$

Here ρ^T is the boundary of the region of small transverse gradients. We obtain ultimately

$$x_0(\rho) = x_c - \frac{1}{4\pi^2}\frac{\rho^{(0)2}}{x_c}\left(\frac{c_\parallel}{c_\perp}\right)^2 \mathrm{li}^{-1}\left(\frac{\rho^T}{\rho^{(0)}}\right)\mathrm{li}^2\left(\left(\frac{\rho}{\rho^{(0)}}\right)^{1/2}\right), \quad (36)$$

where $\mathrm{li}(z)$ is the integral logarithm.

Since $\mathrm{li}(z)$ is positive, the condition $\rho^T/\rho^{(0)} \gtrsim 1.2$, must be satisfied. On the other hand we have $(x_c - x_0)/x_c \sim 1$, already as $\rho \to \rho^{(0)}$. The true boundary of the one-dimensionality region is therefore determined by the condition $\rho_T < \rho^{(0)}$ accurate to terms

$$1 - \frac{\rho_T}{\rho^{(0)}} \ll \exp\left(-\frac{\pi x_c}{2\rho^{(0)}}\frac{c_\perp}{c_\parallel}\right).$$

For $\rho \sim \rho_T$ we have with logarithmic accuracy

$$\left|\frac{\partial x_0}{\partial \rho}\right|_{\rho\sim\rho_T} \lesssim \frac{\rho_T}{x_c}\left(\frac{\rho_T}{\rho_0}\right)^{1/2}\frac{c_\parallel}{c_\perp}, \quad (37)$$

which justifies the use of perturbation theory in terms of small transverse gradients, since $(c_\perp/c_\parallel)^2 (\partial x_0/\partial\rho)^2 \ll 1$. Consequently, if $\alpha \gg 1$ and $x_c \ll \rho_T(\varepsilon_\parallel/\varepsilon_\perp)^{1/2}$ plane sections of size $\rho_T < \rho^*$ are realized on the end faces of the seed (Fig. 1). A numerical estimate confirms this inequality.

We proceed to calculate the tunneling action. Recall that macroscopic (vacuum–vacuum) tunneling takes place over the equal-energy surface $\mathscr{H} = 0$ and at each point of the trajectory the instanton "kinetic" energy is equal to the potential energy, $T = V$ $(l_{\rm eff} = T + V)$. This equality makes it possible, in principle, to express the generalized momentum of the tunneling system in terms of the coordinate x_0 and its derivative $x_0' = \partial x_0/\partial\rho$. The form assumed by us for the tunneling seed surface permits in turn the use of Eqs. (27) and (36) for the $x_0(\rho)$ dependence. In this approach the problem of calculating the tunneling action reduces to the standard one-dimensional problem of quantum mechanics

$$S_{eff} = 2\pi \int \rho\, d\rho \int_{-x_0(\rho)}^{x_0(\rho)} \frac{dx_0}{\dot{x}_0(x_0, x_0')} \times l_{eff}(x_0, x_0'). \quad (38)$$

On the plane section $\rho < \rho_T$ the calculation of the tunneling is elementary:

$$S^{(T)}_{eff} = 2\pi^2 n_f \frac{E_s}{c_\parallel}\int_0^{\rho_T} \rho x_0(\rho)\, d\rho, \quad (39)$$

where $x_0 = x_c$ accurate to $(\rho_T/x_c)^2$. The relative contribution of the breather (16) to the action is of the order of

$$S^{(B)}_{eff} \approx S^{(T)}_{eff}\alpha^3 \frac{\rho_0 d}{\rho_T^2}\left(\frac{\varepsilon_\perp}{\varepsilon_\parallel}\right)^{1/2}\left(\frac{\rho_0}{d}\right)^2 \quad (40)$$

and will be shown to be small compared with $S^{(T)}_{\rm eff}$. Thus, the main qualitative result of the calculation is the existence of plane walls that determine the tunneling action.

For a numerical estimate of the seed parameters we rewrite (39) in the form

$$\frac{S_{eff}}{\hbar} = \frac{E_0/E_T}{(E/E_T - 1)}$$
$$\frac{E_0}{E_T} = \frac{\pi E_s^2 M}{2e\hbar c_\parallel E_T} N_K, \quad (41)$$

where $N_K = \pi\rho_T^2 n_f$ is the number of chains in the plane sections of the seed.

All the quantities in (41) contain the soliton energy E_s, the symbolic expression for which contains the value of the phenomenological parameter of our problem—of the phonon anharmonicity.[11] For a numerical estimate of the actions it is therefore logical to backtrack and attempt to determine from the experimental data E_s, N_K, and all the parameters of the seed.

There are unfortunately no independent measurements of E_s and N_K. One can only assume with large degree of likelihood, following Ref. 1, that 10^{-3} cm $> d > 10^{-4}$ cm. We have then $E_s \approx 1$ K and an estimate of N_K for TaS_3, where $M = 4$, $E_0/E_T = 5$, $E_T = 2.2$ V/cm, $v_F \approx 10^8$ cm/s, and $\hbar\omega/2\Delta \gtrsim 0.1$ yields approximately up to 10^2–10^3 chains. From the expressions for E_T at $\varepsilon_\parallel \approx 10^7$ (Refs. 1 and 12) it follows that $n_f \gtrsim 10^{14}$, $\rho_T \approx 10^{-5}/10^{-6}$ cm.

The smallness of the ratio d/x_c for d on the order of several times 10^{-4} cm determines the range of variation of the electric field $(E - E_T)/E_T \ll 0.7$, in which the thin-wall approximation can be used.

From the condition $x_c \ll \rho_T(\varepsilon_\parallel/\varepsilon_\perp)^{1/2}$ for the existence of the threshold E_T we obtain $\varepsilon_\parallel/\varepsilon_\perp > 10^4$, which is readily met for $\varepsilon_\parallel \sim 10^7$ and $\varepsilon_\perp \lesssim 10^2$. For TaS_3 we have $\alpha > 10$, when $\rho^* \geqslant 0.1d$. A numerical estimate of the correction to the "one-dimensional" action $S^{(B)}_{\rm eff}/S^{(T)}_{\rm eff}$ is of the order of 10^{-2}.

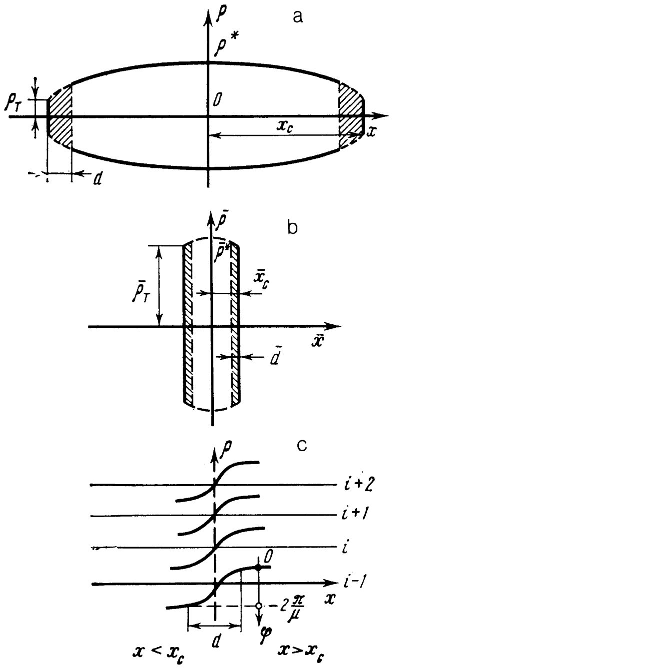

FIG. 1. Schematic representation of the seed: a—in (x,ρ) coordinates, b—in reduced $\bar{x} = x/\varepsilon_\parallel^{1/2}$, $\bar{\rho} = \rho/\varepsilon_\perp^{1/2}$ coordinates, c—structure of seed wall, i—number of chain. The phase soliton is shown on each chain.

CONCLUSION

We have developed a theory of seed production in macroscopic quantum tunneling of a CDW in an above-threshold electric field. This process determines the quantum component of the nonlinear conductivity. A variational procedure was used to calculate the seed shape and to estimate its size. The measured quantities were used to determine the numerical values of the seed parameters and to evaluate the tunneling action.

The seed is cigar-shaped, with a ratio of the critical dimension x_c to the transverse ρ^* on the order of 10. The end faces of the cigar contain small plane sections of size ρ_T, which produce under the condition $x_c \ll \rho_T(\varepsilon_\parallel/\varepsilon_\perp)^{1/2}$ an end-face attraction field E_T that agrees with the field in a parallel-plate capacitor.

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APPENDIX

The generating functional (4) is obtained in the microscopic theory from the experession

$$\mathcal{F}=-i\ln\int D\bar{\Psi}_s D\Psi_s D\Delta D\varphi D\Phi \exp\left(i\int d\mathbf{r}\,dt\,\mathcal{L}\right), \quad \text{(A1)}$$

where $\mathcal{L}$ is the microscopic Lagrangian of a PD (Ref. 11):

$$\mathcal{L}=n_f\Big\{\bar{\Psi}_s\Big[i\sigma_2(\partial_t+ie\Phi)+v_F\sigma_1(\partial_x-ieA) - \sum_{a_\perp}\sigma_2(\mathbf{v}_\perp\nabla_\perp)-\Delta\exp(-i\sigma_3\varphi)-\mu\Delta\exp(i\sigma_3(M-1)\varphi)\Big]\Psi_s - \frac{\Delta^2}{2\lambda}N(0)\,(1+\eta n_f^{-1}(\nabla_\perp\varphi)^2)+\frac{N(0)}{2}\,\frac{\dot{\Delta}^2+\Delta^2\dot{\varphi}^2}{\varpi^2}\Big\}+\frac{(\nabla\Phi)^2}{8\pi}. \quad \text{(A2)}$$

Here ψ_s is a two-component (electron–hole) spinor, s the index of the spin projection, σ a set of Pauli matrices, λ a dimensionless coupling constant, $N(0)$ the density of states on the Fermi level, η the lattice-anisotropy parameter ($\eta < 1$), Φ the electrostatic potential, and $a_\perp = n_f^{-1/2}$.

In the theory of PD the electron–phonon interaction is made up to two contributions: the deformation potential Δ of the optical phonons and the electrostatic self-consistent potnetial Φ. (This corresponds to the standard representation of the electron–phonon interaction matrix element as a sum of a macrofield (Φ) and a microfield (Δ) in the terminology of Ref. 13.) In the calculation of the gound state of a one-dimensional PD it is assumed that $\Delta \gg e\Phi$. Such a scheme describes appropriately real PD, while allowance for Φ by a perturbation method leads in the linear theory to a certain plasma activation of the phason spectrum.[6,11] The small parameters $\varpi/\Delta \ll 1$ and $\Delta/\varepsilon_F \ll 1$ make it possible to separate the contributions of Δ and φ in $\mathcal{F}$ and represent $\mathcal{F}$ in the form[8,11]

$$\mathcal{F}=\mathcal{F}_\Delta+\mathcal{F}_{CDW}, \quad \text{(A3)}$$

where $\mathcal{F}_{\rm CDW}$ is given by Eq. (4).

Solution of tunneling seed problem raises the question of justifying the condition $e\Phi \ll \Delta$, since the charges considered are located on neighboring chains, where $\hat{\varepsilon} = 1$. Let us consider two phase solitons on neighboring chains (Fig. 2) and estimate the Coulomb energy of the interaction.

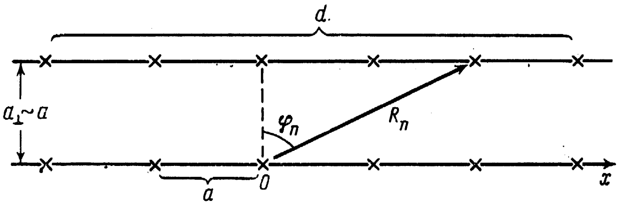

FIG. 2. Scheme for calculating the Coulomb energy of the interaction of two solitons on neighboring chains forming a soliton wall.

Each lattice site has a charge of order $e(a/d)$, and the Coulomb energy in site "0" interacting with the neighboring chain is equal to

$$e\Phi_{12}^{(0)} \sim e^2\left(\frac{a}{d}\right)^2\sum_{n=0}^{N}\frac{1}{R_n}, \quad \text{(A4)}$$

where $N \sim d/a \gg 1$ is the number of sites inside the soliton, $R_n = a/\cos\varphi_n$, and $\tan\varphi_n = n$, i.e.,

$$e\Phi_{12}^{(0)} \approx \frac{e^2}{a}\left(\frac{a}{d}\right)^2\sum_{n=0}^{d/a}\frac{1}{(1+n^2)^{1/2}} \approx e^2\frac{a}{d^2}\ln\frac{d}{a}. \quad \text{(A5)}$$

The total Coulomb energy of the soliton interaction is in this case

$$e\Phi \approx Ne\Phi_{12}^{(0)} \sim \frac{e^2}{d}\ln\frac{d}{a}. \quad \text{(A6)}$$

Accordingly, $e\Phi \sim 10^{-3}\varepsilon_F \sim 10^{-1}\Delta$ and the approximation $e\Phi \ll \Delta$ is justified. Similar reasoning leads to the same estimate for the Coulomb energy of the charge inside a soliton on one chain. The result (A6) remains, naturally, in force also in the continual approximation, when the charge density is given by Eq. (2).

A tensor $\hat{\varepsilon}_{\alpha\beta}$ in Eq. (4) appears in calculations for a crystal containing many chains.[8,11]

[1)] A similar reasoning for an isotropic medium leads to the physically obvious spherically symmetric shape of the seed surface.

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