Published in final edited form as:

Physica B Condens Matter. 2012 June 1; 407(11): 1734–1736. doi:10.1016/j.physb.2012.01.018.

Quantum mechanisms of density wave transport

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Abstract

We report on new developments in the quantum picture of correlated electron transport in charge and spin density waves. The model treats the condensate as a quantum fluid in which charge soliton domain wall pairs nucleate above a Coulomb blockade threshold field. We employ a time-correlated soliton tunneling model, analogous to the theory of time-correlated single electron tunneling, to interpret the voltage oscillations and nonlinear current-voltage characteristics above threshold. An inverse scaling relationship between threshold field and dielectric response, originally proposed by Grüner, emerges naturally from the model. Flat dielectric and other ac responses below threshold in NbSe₃ and TaS₃, as well as small density wave phase displacements, indicate that the measured threshold is often much smaller than the classical depinning field. In some materials, the existence of two distinct threshold fields suggests that both soliton nucleation and classical depinning may occur. In our model, the ratio of electrostatic charging to pinning energy helps determine whether soliton nucleation or classical depinning dominates.

Keywords

Charge density wave; spin density wave; soliton; quantum tunneling

1. Time-correlated soliton tunneling model

Our understanding of cooperative quantum tunneling has undergone significant advances since the 1960's. The tunneling Hamiltonian matrix element proposed by Bardeen [1] led to Josephson's theory [2] of coherent tunneling of superconducting electron pairs. Coherent Josephson tunneling has also been reported for Bose-Einstein condensates [3]. The widely cited "Fate of the False Vacuum" papers [4,5] discuss quantum instability of a scalar field $\phi(\mathbf{r})$ in a double-well potential. In quantum field theory, the term "vacuum" refers to a minimum energy state.

In this paper, ϕ represents the phase of a density wave. If ϕ sits in the higher metastable well ('false vacuum') it is unstable to decay by tunneling into the lower potential well, nucleating a bubble of 'true vacuum' bounded by charge soliton domain walls. The charge density wave (CDW) is an anisotropic (quasi-1-D) correlated electron-phonon system [6] in which quantum interference between right- and left-moving electron states creates a charge modulation, $\rho_k(x, t) = \rho_0(x, t) + \rho_1 \cos[2k_F x - \phi_k(x, t)]$, along each (k^{th} out of N) parallel chain or transverse wavevector. A spin density wave (SDW) is equivalent to two out-of-

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phase CDWs for the spin-up and spin-down subbands. If the phases are correlated, $\varphi_k \approx \varphi$, then the net charge per unit length, averaged over several wavelengths, is given by: $\langle \rho(x,t) \rangle = (Q_0/2\pi) \varphi(x,t)/x$, where $Q_0=2Ne\rho_c$ and ρ_c is the condensate fraction. An applied field E thus couples to kinks rather than the phase, and the apparent coupling to φ comes from integrating by parts and throwing away the boundary conditions. Crucially, any charged kinks produce their own electric field, which contributes an electrostatic component to the potential energy. The density wave (DW) pinning energy is periodic in φ and can be idealized as a sine-Gordon potential, $\propto 1 - \cos\varphi$, in the simplest model.

Dielectric, *ac* conductivity, and mixing responses [7–9] of NbSe₃ and TaS₃, some at temperatures above 200 K, are nearly bias-independent below the threshold field E_T for nonlinear transport. These results corroborate small CDW phase displacements [10] and contradict classical predictions [11–13] of divergent dielectric response, suggesting that E_T (measured) $\ll E_T$ (classical). Quantized states in CDW microcrystals [14] and $\hbar/2e$ Aharonov-Bohm oscillations in the CDW magneto-conductance of NbSe₃ crystals with columnar defects [15] and TaS₃ rings [16] further reveal cooperative quantum behavior. The observed $\hbar/2e$, rather than $\hbar/2Ne$ period predicted [17] for N parallel chains, suggests coherent Josephson-like tunneling of microscopic entities of charge $2e$ within the condensate, as the quantum fluid flows through a tiny barrier, rather than tunneling of a massive object. Unlike macroscopic quantum tunneling, Josephson tunneling can occur at all temperatures below the condensation temperature (Peierls temperature for CDWs), which for NbS₃ is well above room temperature [18].

The quantum picture discussed here interprets the threshold field and coherent oscillations above threshold as due to Coulomb blockade [19] and time-correlated tunneling of microscopic quantum solitons that condense into soliton domain walls [20–22]. Once fully nucleated, the domain walls (Fig. 1) carry charges $\pm Q_0$. These produce an internal field, $E^*=Q_0/\varepsilon A$, where A is the crystal's cross-sectional area. The difference in electrostatic energies, $\frac{1}{2} \varepsilon (E \pm E^*)^2 - \frac{1}{2} \varepsilon E^2$, with and without soliton pairs is positive when the applied field E is less than a Coulomb blockade threshold, $E_T = \frac{1}{2} E^* = Q_0/2\varepsilon A$, which can be much less than the classical depinning field. However, when $E > E_T$, or $\theta = 2\pi E/E^* > \pi$, the formerly 'true vacuum' becomes a metastable state or 'false vacuum,' as illustrated in Fig. 2. Similar $\theta = \pi$ instabilities, where θ represents the vacuum angle, have been proposed for spontaneous *CP* violation [23,24] and several condensed matter systems, including topological insulators [25] and the quantum Hall effect [26].

Like the classical depinning field E_{cl} , E_T scales as n_i^2 for a weakly pinned sample, n_i being the impurity concentration. This can be seen by examining the Grüner relation between dielectric response and threshold field, which for the simplest classical model is given by [6]: $\varepsilon E_{cl} = 4\pi en_{ch}\rho_c$, where ε is the low-frequency dielectric response at zero bias and $n_{ch} = N/A$. The Coulomb blockade threshold $E_T = Q_0/2\varepsilon A$ leads to a similar relationship: $\varepsilon E_T = en_{ch}\rho_c$, with the result, $E_T = E_{cl}/4\pi$, which scales as n_i^2 for a DW weakly pinned by impurities. Screening by normal carriers, both thermally activated and due to incomplete Peierls gaps in materials such as NbSe₃, further enhance ε and reduce the ratio E_T/E_{cl} . For a fixed n_i , the temperature dependence of ε leads (inversely) to the observed [27] temperature dependence of E_T .

The 'vacuum angle' θ is related to total displacement charge Q by: $\theta = 2\pi(Q/Q_0)$. This contributes an electrostatic energy, $Q^2/2C$, which is either enhanced or reduced by the internal field from a kink-antikink pair within which the phase is advanced. The potential energy per unit length of the k^{th} chain or transverse wavevector can thus be written as [21–22]:

$$u(\varphi_k) = u_p[1 - \cos\varphi_k] + u_E[\theta - \varphi_k]^2, \quad (1)$$

where the first term is the pinning energy and the second, quadratic term is the electrostatic contribution. The inclusion of both terms clearly delineates a quantum threshold, which is much smaller than the classical depinning threshold when $u_E \ll u_p$. When $\theta > \pi$, the state with $\varphi_k \sim 2\pi$ becomes the lowest energy state, as illustrated in figure 2 (left). Thus, $\theta = \pi$ demarcates the boundary above which a dynamical phase transition via quantum decay of the ‘false vacuum’ becomes possible. Below threshold when $\theta < \pi$, in the limit $\alpha \equiv u_E/u_p \ll 1$ we find (setting $\varphi_k = \varphi$ and $u/\varphi = 0$, and using $\sin\varphi \approx \varphi$) that $\varphi \cong [u_E/(u_E + u_p)]\theta \approx \alpha\theta \sim 0$, leading to a small phase displacement and relatively flat dielectric response below threshold.

The right side of figure 2 shows plots of u vs. θ , obtained by minimizing the energy for $\varphi_k \approx \varphi \sim 2\pi n$. A voltage across the contacts induces a displacement charge Q . The charging energy, $\propto (\theta - 2\pi n)^2$ in Fig. 2, can be expressed (for N parallel chains) in terms of total displacement charge as $U_C = (Q - nQ_0)^2/2C$, showing a clear analogy to time-correlated single-electron tunneling (SET) in Coulomb blockade tunnel junctions [28]. The origin of the narrow-band noise, coherent voltage or current oscillations, and mode locking with an ac source thus becomes clear in this context.

In order to simulate DW dynamics above threshold, we employ a model that includes a shunt resistance R in parallel with a capacitive tunnel junction representing soliton tunneling, by analogy to time-correlated SET [28]. Details of these simulations will be discussed elsewhere. The phases φ_k tunnel coherently into the next well as each parabola in Fig. 2 crosses the next at the instability points $\theta = 2\pi(n + 1/2)$. We represent the amplitudes for the system to be on branches 0 and 1 (more generally n and $n+1$) as $\psi_{0,1} = \rho_{0,1} \exp[i\delta_{0,1}]$, where $\rho_{0,1} = N_{0,1}/N$ is the fraction of chains or transverse wavevectors on branch 0 or 1. These are coupled via a tunneling Hamiltonian matrix element T with a Zener-like dependence $\propto F \exp[-F_0/F]$ on the force F , which is proportional to the difference in energies between the two branches for a specific value of θ . Following Feynman’s treatment of the Josephson junction [29], the time-evolution of ψ_0 and ψ_1 is described using the Schrödinger equation, viewed as the “classical” equation of motion for the system:

$$i\hbar\partial\psi_{1,0}/\partial t = U_0\psi_{1,0} + T\psi_{0,1}. \quad (2)$$

The simulation results, to be discussed elsewhere, yield excellent quantitative agreement with measured coherent voltage oscillations and current-voltage characteristics in NbSe₃. Moreover, the model explains the existence of more than one threshold field, as observed in some materials [30,31]. The two major thresholds emerge naturally, provided the nucleated soliton conductance is sufficiently small for θ to be treated quasi-statically, i.e. $\theta = \pi\epsilon E/\epsilon_1 E_T$, where $\epsilon_1 = \epsilon(E \approx E_T)$. We interpret the low- and high-field thresholds as due to soliton nucleation and classical depinning, respectively. The quantum instability occurs when $\theta \sim \pi$, while the classical instability occurs when $\theta \sim \theta_c(\alpha) \cong \alpha^{-1} + \pi/2$ in the limit $\alpha = u_E/u_p \ll 1$. The data showing flat dielectric and other ac responses suggest $\alpha \ll 1$, where soliton nucleation is the dominant mechanism. However, some crystals and temperature ranges suggests a higher u_E/u_p , which enables both a low-field soliton nucleation threshold and high-field classical depinning threshold. Finally, in some materials at low temperatures [30,31], the normal carriers become frozen out and result in a relatively low ϵ and sufficiently high u_E/u_p for classical depinning to dominate.

2. Discussion

The issue of whether DW transport is a high temperature cooperative quantum phenomenon is potentially of major significance. Areas of broad scientific impact include improved understanding of correlated electron systems, tunneling in quantum cosmology, spontaneous *CP* violation [23,24], and in some materials (e.g. NbS₃ for which $T_P \sim 360$ K [18]), the possibility of macroscopic quantum effects at biological temperatures. Finally, understanding of the quantum behavior of solitons could lead to topologically robust forms of quantum information processing.

Acknowledgments

The authors acknowledge support by R21CA133153 from NIH (NCI) and by ARRA supplement: 3 R21 CA133153-03S1 (NIH, NCI). Additional support was provided by the State of Texas through the Texas Center for Superconductivity at the University of Houston.

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Fig. 1.

Top. Density wave phase vs. position, showing production of a soliton-antisoliton domain wall pair. **Bottom.** Model of density wave capacitance showing nucleated domain walls moving toward the contacts. The applied field E partially or completely cancels the internal field E^* . The distance l , soliton width $\lambda_0 = c_0/\omega_0$, where c_0 and ω_0 are the phason velocity and pinning frequency, respectively, and crystal thickness are exaggerated for clarity.

Figure 2.

Left. Potential energy vs. ϕ for two values of θ , in which the many degrees of freedom are illustrated schematically. Tunneling can only occur if $\theta > \pi$ ($E > E_T$), when the phases ϕ_k tunnel coherently into the adjacent well. **Right.** Potential energy vs. θ , in which the phases $\phi_k \approx \phi$ are sitting in various potential minima, $\phi \sim 2\pi n$.