Quantum dynamical phase transition in the soliton nucleation model of density wave transport

J H Miller, Jr.
Department of Physics and Texas Center for Superconductivity,
University of Houston, 4800 Calhoun, Houston, Texas 77204-5005, USA
E-mail: jhmiller@uh.edu

Abstract. In the sine-Gordon model of a pinned density wave (DW), the electrostatic energy generated by charged solitons (S) and antisolitons (Ŝ) leads to a Coulomb blockade threshold field $E_T$ for quantum $S\bar{S}$ pair creation. This field can be far smaller than the classical depinning field, since the quantum instability occurs as soon as the formerly lowest energy potential well rises to become a metastable well, or “false vacuum.” The analogy to time-correlated single electron tunnelling, as well as broader implications of the proposed tunnelling process, are briefly discussed.

1. Introduction

The charge density wave (CDW) is a highly anisotropic correlated electron-phonon system in which quantum interference between right- and left-moving electron states leads to a divergent $2k_F$ Lindhard response and softening of the $2k_F$ phonon mode [1]. Below the Peierls transition, this results in a lattice distortion and charge modulation $\rho(x, t) = \rho_0(x, t) + \rho_1 \cos[2k_Fx - \phi(x, t)]$ along the main axis of the needle-like crystal. Here $\rho_0(x, t)$ contains the background charge of the condensed electrons and any excess or deficiency of charge $\propto \partial \phi / \partial x$. A Peierls gap $2\Delta(T)$ opens up at the Fermi surface, and its temperature dependence resembles that of the BCS gap in a superconductor. The electron-hole condensate is coupled to a macroscopic occupation of $2k_F$ phonons, which increases the electron effective mass by the Fröhlich mass ratio, $\mu = M/m$. A spin density wave (SDW) is equivalent to two out-of-phase CDWs for the spin-up and spin-down subbands, and is thought to be mediated by electron-electron interactions. In either case, the DW wavelength is given by $\lambda_{DW} = \pi h / p_F = \pi / k_F$.

The Peierls gaps at $\pm k_F$ can be displaced in momentum space in an unpinned DW, resulting in a DW current $\propto \partial \phi / \partial t$. Its fermionic representation resembles a Luttinger liquid [2] of dressed electrons (quantum solitons), except the Fermi velocity gets replaced by the phason velocity $c_0 = \mu^{-1/2}v_F$ [3] and a real DW comprises many parallel chains. When pinned by impurities, a DW can still transport a current provided the applied electric field exceeds a threshold $E_I$. Displacing the DW by one wavelength (advancing $\phi$ by $2\pi$) returns the system to its original state, except for charge displaced between contacts, so the pinning energy is a periodic function of phase. Observations of narrow-band noise and coherent oscillations [1] suggest that a sine-Gordon model can provide a suitable idealized framework, provided electrostatic interactions between charged kinks are taken into account.
2. Coulomb blockade threshold field and time-correlated soliton tunnelling

The pivotal experiments on NbSe$_3$ by Monceau et al [4] revealed Zener-like behaviour of the form: $J_{cdw} \sim E \exp[-E_0/E]$. The characteristic field $E_0$ proved far too small to represent Zener tunnelling of normal electrons across the Peierls gap. This observation motivated Bardeen [5] to propose coherent Zener tunnelling of condensed electrons through a tiny “pinning gap” created by impurity scattering which, unlike the Peierls gaps, would be fixed in momentum space at $\pm k_F$. An instanton picture, proposed by Maki [6], interprets the Zener-like behavior in terms of quantum nucleation of soliton-antisoliton pairs. Later experiments [7] revealed a sharp threshold field $E_T$ for CDW transport, which Bardeen interpreted [8] in terms of a maximum tunnelling distance. Impedance and mixing experiments [9-11] showing agreement with photon-assisted tunnelling theory, and $\hbar/2e$ quantum interference in the CDW magnetoconductance of NbSe$_3$ crystals [12] with columnar defects and TaS$_3$ rings [13], provide compelling evidence of their quantum character.

Another interpretation of the threshold field [14], as an S-$\bar{S}$ pair-creation threshold due to Coulomb blockade [15], is motivated by Coleman’s paper on the massive Schwinger model [16]. A pair of soliton ($S$) and antisoliton ($\bar{S}$) domain walls [17] carry charges $\pm Q_0 = \pm 2Ne$ (in a fully condensed system counting both spins) where $N$ is the number of parallel chains. Like a parallel plate capacitor, these produce an internal electric field of magnitude, $E^* = Q_0/\epsilon A$, where $\epsilon$ is the dielectric constant and $A$ is the cross-sectional area, as shown in figure 1. When an external field $E$ is applied, the difference in electrostatic energies of a state with a pair of separation $l$ and that of the ‘vacuum’ with no pair is: $\Delta U = \frac{1}{2} \epsilon A [(E \pm E^*)^2 - E^2] = Q_0 \frac{1}{2} [(E^* \pm E)^2 - E^2]$, which is positive when $|E| < \frac{1}{2} E^*$. Conservation of energy thus forbids pair production for fields less than the Coulomb blockade threshold, $E_T \equiv \frac{2}{3} E^* = Q_0/2eA \sim Ne/eA$, which can be substantially smaller than the classical depinning field. The experimentally observed scaling law [1], $\epsilon E_T \sim e n_{ch}$ (for a fully condensed system), where $n_{ch} = N/A$, arises naturally in this model.

Figure 1. Top. Density wave phase vs. position, showing the production of a soliton-antisoliton domain wall pair.

Bottom. Model of density wave capacitance, in which the nucleated domain walls are moving toward the contacts. The applied field $E$ partially or completely cancels the internal field $E^*$. The distance $l$, soliton width $\lambda_0 = c_0/\omega_0$, and crystal thickness are greatly exaggerated for clarity.

If the DW phase is fixed at zero at the contacts or at $\pm \infty$, advancing the phase by $\phi$ in the middle creates charged kinks that produce an internal electric field: $E_\phi = (E^*/2\pi)\phi$. $E^*$ can also be written as $E^* = 2e/\epsilon A_{ch}$ (counting both spins), where $A_{ch}$ is the cross-sectional area of a single chain, since $A = N \epsilon A_{ch}$. If an applied field, represented by a dimensionless parameter $\theta = 2\pi (E/E^*) = \pi (E/E_T)$, partially cancels the internal field $E_\phi$, this yields an electrostatic energy proportional to $(\theta - \phi)^2$. The Hamiltonian for a single chain can then be written as:
\[ H = \int_{-L/2}^{L/2} dx \left\{ \sum_{\sigma = \uparrow, \downarrow} \left[ \frac{1}{2D} \Pi_{\sigma}^2 (x) + \frac{1}{2} D c_0^2 \left( \frac{\partial \phi_{\sigma}(x)}{\partial x} \right)^2 + D \omega_0^2 \left[ 1 - \cos \phi_{\sigma}(x) \right] \right] \right\} \]

\[ U \cos[\phi_{\uparrow}(x) - \phi_{\downarrow}(x)] + u_E (\theta - \phi(x))^2 \right\} \]

where \( \phi_{\sigma} \) represent phases corresponding to the two spin sub-bands, \( \phi \equiv (\phi_{\uparrow} + \phi_{\downarrow})/2 \), \( D = \frac{\mu h}{4\pi v_F} \), \( \omega_0 \) is the pinning frequency, \( \Pi_{\sigma}(x) = D \frac{\partial \phi_{\sigma}(x)}{\partial t} \) is the canonical momentum density, and \( u_E = \frac{e^2}{2\pi^2 \epsilon_{\infty}} \). The minus sign is appropriate for a CDW in the interaction term, \( \mp U \cos[\phi_{\uparrow} - \phi_{\downarrow}] \), since this tends to keep the two spin sub-bands in-phase, whereas the + sign applies to an SDW. Defining \( u_p \equiv D \omega_0^2 \) and assuming \( U \gg u_p \), we see that the interaction term tends to constrain the phases along a saddle point in a plot of potential energy vs. \( \phi_{\uparrow} \& \phi_{\downarrow} \)(focusing for the moment on the CDW) such that \( \phi_{\uparrow} \approx \phi_{\downarrow} \approx \phi \), which simplifies the remaining potential energy contributions to:

\[ U[\phi] = \int_{-L/2}^{L/2} dx \left\{ 2u_p \left[ 1 - \cos \phi(x) \right] + u_E \left( \theta - \phi(x) \right)^2 \right\} . \]

The usual linear coupling \( \sim -\theta \phi \) is implicitly contained in the quadratic energy term, which also includes electrostatic contributions \( \sim \phi^2 \) and \( \theta^2 \). The inclusion of both pinning and electrostatic contributions clearly delineates a quantum threshold, which is much smaller than the classical depinning threshold when \( u_E \ll u_p \). Setting \( F \propto -\partial \phi / \partial \phi = 0 \), in the limit \( \alpha \equiv u_E / u_p < 1 \) we find (using \( \sin \phi \approx \phi \)) that \( \phi \approx \left[ u_E / (u_E + u_p) \right] \theta \approx \alpha \theta \approx 0 \) when \( \theta < \pi \). When \( \theta > \pi \), the state with \( \phi \approx 2\pi \) 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.

The right side of figure 2 shows plots of \( u \) vs. \( \theta \), obtained by minimizing the energy for \( \phi \approx 2\pi n \). An applied field induces a displacement charge \( Q \) across the contacts, which is related to \( \theta \) by: \( \theta = 2\pi (Q / Q_0) \). Suppose the system is initially sitting in the \( \phi \sim 0 \) potential minimum. When \( \theta \) exceeds \( \pi \), what was once the ground state (true vacuum) now becomes a metastable state (false vacuum) as the solid line in the right side of figure 2 crosses above the dashed line. One or more bubbles of true vacuum then nucleate, in which \( \phi \) advances by \( 2\pi \) with soliton-antisoliton domain walls at the boundaries, and each bubble rapidly expands as the electric field drives the oppositely charged soliton domain walls toward the contacts (figure 1). The total charging energy, \( \propto (\theta - 2\pi n)^2 \) in figure 2, can be re-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 tunnelling in Coulomb blockade tunnel junctions. 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.
3. Discussion

Observations of flat, essentially bias voltage-independent dielectric and other ac response data below threshold [11] suggest that many DW samples show little phase displacement below threshold and are thus in the region where $\alpha = u_E/u_0 \ll 1$ (recalling that $\phi \approx \alpha \theta$). This is consistent with the interpretation that, for these samples, the Coulomb blockade threshold for soliton pair production is well below the classical depinning field. Dias and Lemos [18] propose that the probability of nucleating a soliton domain wall pair by tunnelling is determined by the mass-energy (or action) density of a domain wall rather than the total mass-energy, and is therefore scale invariant – i.e. independent of the transverse dimensions. An alternative argument [3,17] is that each domain wall can be viewed as a condensate of microscopic quantum solitons that tunnel coherently within a system with only one thermal degree of freedom, as in Josephson tunnelling. This approach suggests that, rather than computing the total Euclidean action or “bounce,” the tunnelling Hamiltonian matrix element concept should be extended to other systems, such as quantum solitons. A growing body of literature proposes that the entire universe came into existence through a quantum nucleation process, and subsequently tunnelled hundreds or thousands of times into successively lower potential wells, in order to explain why the cosmological constant is small and positive (e.g. see [19]). This being the case, it would make sense to determine whether large scale quantum tunnelling can occur in the laboratory. Moreover, any possibility of observing quantum interference in rings of NbS$_3$, which undergoes a Peierls transition above room temperature, could be of practical importance for biomedical and other applications.

4. References

[1] Grüner G 1994 *Density Waves in Solids* (Reading, MA: Addison-Wesley)
[2] Artemenko S N and Remisov S V 2005 *Phys. Rev. B* 72 125118
[3] Maiti A and Miller J H Jr 1991 *Phys. Rev. B* 43 12205
[4] Monceau P, Ong N P, Portis A M, Meershaut A and Rouxel J 1976 *Phys. Rev. Lett.* 37 602
[5] Bardeen J 1979 *Phys. Rev. Lett.* 42 1498
[6] Maki K 1977 *Phys. Rev. Lett.* 39 46
[7] Fleming R M and Grimes C C 1979 *Phys. Rev. Lett.* 42 1423
[8] Bardeen J 1980 *Phys. Rev. Lett.* 45 1978
[9] Miller J H Jr, Richard J, Tucker J R, and Bardeen J 1983 *Phys. Rev. Lett.* 51 1592
[10] Miller J H Jr, Thorne R E, Lyons W G, Lyding J W, Tucker J R and Bardeen J 1985 *Phys. Rev. B* 31 5229
[11] Miller J H Jr 1985 *Quantum Tunneling of Charge Density Waves in Quasi-One-Dimensional Conductors* (PhD Dissertation, University of Illinois at Urbana-Champaign)
[12] Latyshev Yu I, Laborde O, Monceau P and Klaumünzer S 1997 *Phys. Rev. Lett.* 78 919
[13] Tsubota M, Inagaki K and Tanda S 2009 *Physica B* 404 416
[14] Krive I V and Rozhavsky A S 1985 *Solid State Commun.* 55 691
[15] Miller J H Jr, Ordóñez C and Prodan E 2000 *Phys. Rev. Lett.* 84 1555
[16] Coleman S 1976 *Ann. Phys., NY* 101 239
[17] Miller J H Jr, Cárdenas G, Garcia-Perez A, More W and Beckwith A W 2003 *J. Phys. A: Math. Gen.* 36 9209
[18] Dias O J C and Lemos J P S 2001 *J. Math. Phys.* 42 3292
[19] Steinhardt P J and Turok N 2006 *Science* 312 1180

Acknowledgments

The author gratefully acknowledges the assistance of Divya Pamaraj in preparing figure 2 and financial support from NIH (NCI & NHLBI) R21CA133153, NIH (NCI) ARRA supplement 3R21CA133153-03S, and the State of Texas through the Texas Center for Superconductivity at the University of Houston and the Norman Hackerman Advanced Research Program.