Quantum Field Theory of the Pinned Density Wave

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Abstract

A model is discussed in which an electric field induces quantum nucleation of soliton-antisoliton pairs in a pinned charge or spin density wave. Coulomb blockade prevents pair creation until the electric field exceeds a sharp threshold value, which can be much smaller than the classical depinning field. We calculate the vacuum state energy and expectation value of the phase $\phi$, which is treated as a quantum scalar field. We find that the phase can also be much smaller, below threshold, than predicted by classical “sliding” density wave models.

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Charge and spin density waves are examples of spontaneous symmetry breaking, in which pairs of electrons and holes condense into a new ground state. A charge density wave (CDW) forms in a linear chain compound when the electronic charge density becomes modulated: \( \rho(x) = \rho_0(x) + \rho_1 \cos[2k_Fx - \phi(x,t)] \), where \( \phi \) is the phase. A spin density wave (SDW) has a modulated spin density, \( \Delta S(x) = \Delta S_0 \cos[2k_Fx - \phi(x,t)] \), and is equivalent to two out-of-phase CDWs for the spin-up and spin-down subbands. Although pinned by impurities, a density wave (DW) can transport a current when an applied field exceeds a threshold value \( E_T \). The simplest model of a pinned DW is a sine-Gordon (s-G) model, in which the "vacuum states" are the \( 2\pi n \) minima about which a DW would oscillate at the pinning frequency \( \omega_0 \) in the absence of dissipation. Finite wavelength modes, or phonons, can propagate at the phason velocity, \( c_0 = \mu^{-1/2}v_F \), where \( \mu = M_F/m_e \) is the Fröhlich mass ratio.

The Hamiltonian for a pinned DW, including Coulomb interactions, can be written as:

\[
H = \int dx \left\{ \frac{\pi^2}{2D} + \frac{1}{2} Dc_0^2 \left( \frac{\partial \phi}{\partial x} \right)^2 + D\omega_0^2 \left[ 1 - \cos \phi \right] + u_E \left[ \phi - \theta \right]^2 \right\},
\]

where \( D = \frac{\mu h}{4\pi v_F} \) (per spin per chain), and the canonical momentum density is given by \( \pi = D\partial_t \phi \). The last term in Eq. (1), introduced by Krive and Rozhavsky, is the electrostatic energy density \( \frac{1}{2} \varepsilon (E_{int} \pm E)^2 \) due to the applied field \( E \) and the internal fields \( E_{int} \sim - (\phi/2\pi) E^* \) generated by phase variations. Here, \( E^* \) represents the internal field produced by a \( 2\pi \) soliton-antisoliton (S-S') pair (Fig. 1(a)), \( u_E = \frac{1}{2} \varepsilon A (E^*/2\pi)^2 \) is the electrostatic energy density, \( \theta = 2\pi E/E^* \) is proportional to the applied electric field, and \( \phi \) is measured with respect to its value at \( x = \pm \infty \). The above Hamiltonian is equivalent to the bosonic form of the massive Schwinger model, as discussed by S. Coleman. A topological soliton (antisoliton) of width \( \lambda_\phi = c_0/\omega_0 \sim 1\mu m \) carries a charge \( \mp e^e = \mp n' e \) per spin-chain, where \( n' \) is the condensate fraction. A soliton-antisoliton (S-S') pair can nucleate by quantum tunneling when an electric field is applied. In a related picture, a pair is created when a quantum soliton Zener tunnels through a "Bardeen pinning gap."

The electrostatic (Coulomb) energy of the S-S' pair introduces a sharply defined threshold field for pair creation. Figure 1(a) shows an S-S' pair, displaying the phase \( \phi \) and excess charge density \( \delta \rho = - (e^*/2\pi) \partial_x \phi \) as functions of position. The pair, analogous to a parallel plate capacitor of separation \( L \) and cross-sectional area \( A \) per chain (per spin), produces an internal field of magnitude \( E^* = e^*/\varepsilon A \). The enormous dielectric constant, \( \varepsilon \sim 10^8 \varepsilon_0 \), may include an intrinsic contribution \( \varepsilon_{DW} \) from the pinned DW, as well as a substantial contribution \( \varepsilon_s \) due to screening by the normal carriers. When an external field \( E \) is applied, the difference between the electrostatic energy of a state with a pair and that of the vacuum is given by

\[
\Delta U = \frac{1}{2} \varepsilon A L \left[ (E \pm E^*)^2 - E^2 \right] = e^* L \left[ \frac{1}{2} E^* \pm E \right].
\]

Note that \( \Delta U \) is positive.
when $|E| < \frac{1}{2} E^*$, so conservation of energy forbids the vacuum to produce a pair for fields less than a threshold value $E_T \equiv \frac{1}{2} E^*$ (corresponding to $\theta = \pi$). The threshold voltage across a region of length $L$ will thus be $e^*/2C$ (where $C = \varepsilon A/L$), by analogy to Coulomb blockade in tunnel junctions. Above threshold, the S-S' nucleation and annihilation events will become correlated in time, by analogy to time-correlated single electron tunneling (Fig.1(b)).

This model has at least two important consequences. First, the threshold field for pair creation, $E_T (= e^*/2\varepsilon A)$, can be much smaller than the classical depinning field in the s-G model, $E_c \equiv 2\pi D\omega_0^2/e^*$, provided $u_E < D\omega_0^2$. Secondly, the phase displacement $\phi$ below threshold can also be much smaller than either the classical s-G prediction, $\phi = \sin^{-1}(E/E_c)$, or the substantial phase displacements predicted by more realistic classical models. A growing body of evidence demonstrates that the CDW phase displacements below threshold are extremely small for a wide range of temperatures in NbSe$_3$ and TaS$_3$—a fact which cannot readily be interpreted classically. This evidence includes: (1) the observed $2^\circ$ displacement of CDW phase in NbSe$_3$, as determined by NMR experiments, when $E = (3/4) E_T$, (2) the complete absence of any increase in CDW dielectric response (“critical polarization”) below threshold in NbSe$_3$ and TaS$_3$, in serious contradiction with classical predictions, and (3) most recently, the observed absence of any change in CDW wavevector $Q$ near the contacts below threshold.

The primary goals of this paper are, treating the phase $\phi$ as a scalar quantum field, to calculate the vacuum state energy, $\varepsilon$, and expectation value of the phase $\langle \phi \rangle$ in the metastable regime. In order to evaluate $\varepsilon$ and $\langle \phi \rangle$, we follow Coleman and employ a variational method, choosing the trial states to be coherent states. Such a choice is especially appropriate for a density wave, whose actual ground state (of the 3-D system) is, in fact, a coherent state. A CDW, for example, consists of a condensate of electron-hole pairs coupled to a condensate of $2k_F$ phonons, which are bosons. Such a ground state is characterized by a well-defined expectation value $\langle \phi \rangle$. It is pointed out in Ref. [15] that a piece of every term in the perturbation series expansion is effectively included by this variational approach.

Rescaling $(ct, x) = (x^0, x^1) \to \frac{1}{Dc_0^2} (x^0, x^1)$, the Hamiltonian Eq. (1) now reads:

$$H = \int dx^1 N_{m_0} \left\{ \frac{1}{2} \left[ \left( \frac{\partial \phi}{\partial x^0} \right)^2 + \left( \frac{\partial \phi}{\partial x^1} \right)^2 \right] + U (\phi) \right\} = \int dx \, \mathcal{H} (x),$$

with

$$U (\phi) = \omega^2 [1 - \cos \phi] + \frac{1}{2} m_0^2 (\phi - \theta)^2,$$

where $\omega^2 = D^2 c_0^2 \omega_0^2$, $m_0 \equiv [2Dc_0^2 u_E]^{1/2}$ and $N_{m_0}$ means normal order with respect to $m_0$. The parameter $m_0$ can be interpreted as a “free field” mass in the absence of the washboard pinning potential.
For the theory defined by Eq. (2), all ultraviolet divergences can be removed by normal-ordering in the interaction picture. However, variational calculations are carried out in the Schrödinger picture. Nevertheless, as pointed out in Ref. [15], one can still define a normal order \( N_m \) with respect to an arbitrary mass parameter \( m \). Following Ref. [15], the Hamiltonian density can be re-written as:

\[
H = N_m [H_0 + U(\phi)] = N_m [H_0 + U(\phi, m)]
\]  

(4)

where \( H_0 \) is the kinetic piece of the Hamiltonian Eq. (2) and \( U(\phi, m) \) is defined by:

\[
U(\phi, m) = \exp \left[ \frac{1}{8\pi} \ln \left( \frac{m_0^2}{m^2} \right) \frac{d^2}{d\phi^2} \right] U(\phi) + \frac{(m^2 - m_0^2)}{8\pi}.
\]  

(5)

Now, it is straightforward to calculate the expectation value of the Hamiltonian density on the vacuum states appropriate to free fields of arbitrary mass \( m \), which is given by the free coefficient of Eq. (5). Obviously, this class of states is not rich enough to be a good trial for the variational method. In order to ensure that \( \langle \phi \rangle \) is well defined and to allow nonzero values of \( \langle \phi \rangle \), one introduces a family of coherent states, \( | \xi(x), p(x) \rangle \), labeled by two arbitrary functions of space: \( \xi(x) \) and \( p(x) \). Such coherent states have the property that, for any function of \( \pi(x) \) and \( \phi(x) \), \( F(\pi(x), \phi(x)) \), the expectation value is given by:

\[
\langle \xi(x), p(x) | N_m F \left( \hat{\pi}(x), \hat{\phi}(x) \right) | \xi(x), p(x) \rangle = F(p(x), \xi(x)).
\]  

(6)

These are used as trial states to minimize the expectation value \( \langle \mathcal{H} \rangle \). Using Eq. (4) and the property Eq. (6) we have then:

\[
\langle \xi(x), p(x) | \mathcal{H}(x) | \xi(x), p(x) \rangle = \frac{1}{2} p(x)^2 + \frac{1}{2} (\partial_t \xi(x))^2 + U(\xi(x), m).
\]  

(7)

Choosing \( p \equiv 0 \) and \( \xi(x) = \xi(\langle \phi \rangle) = \text{const.} \) we minimize the first two terms. The energy density becomes:

\[
\varepsilon = \omega^2 \left[ 1 - \left( \frac{m^2}{m_0^2} \right) \frac{1}{8\pi} \cos \xi \right] + \frac{m_0^2}{2} (\xi - \theta)^2 - \frac{m_0^2}{8\pi} \ln \left( \frac{m^2}{m_0^2} \right) + \frac{m^2 - m_0^2}{8\pi}.
\]  

(8)

Minimizing \( \varepsilon \) with respect to \( m \) and \( \xi \), one obtains the following self-consistency equations:

\[
\begin{align*}
\frac{m^2}{m_0^2} &= \frac{\omega^2}{m_0^2} \left( \frac{m^2}{m_0^2} \right)^{\frac{1}{8\pi}} \cos \xi + 1, \\
\frac{\omega^2}{m_0^2} \left( \frac{m^2}{m_0^2} \right)^{\frac{1}{8\pi}} \sin \xi + \xi - \theta &= 0.
\end{align*}
\]  

(9)
We have also derived the above self-consistency equations by extending the mean field approximation first developed by Glimm, Jaffe, and Spencer\textsuperscript{16} for quartic interactions and then extended by Imbrie\textsuperscript{17} to polynomial interactions. Details of our calculations will be reported elsewhere.\textsuperscript{18}

Equations (9) enable one to determine both the mass-ratio $m/m_0$ and phase displacement $\xi \equiv \langle \phi \rangle$ self-consistently in the metastable regime. Figure 2 shows the resulting plots of $\langle \phi \rangle$ vs. $\theta$ (where $\theta$ is the normalized applied electric field) for several different values of the parameter $\tau = \frac{2u_E}{D\omega_0}$, which represents the ratio of the electrostatic energy to the pinning energy. The solid lines through the symbols represent the lowest energy states. Recall that S-S' pair creation can occur only when $\theta > \pi$ (i.e. $E > E_T = E^*/2$). If $\theta = \pi$ was taken to represent the classical depinning field (i.e. if $E_T$ was assumed to be equal to $E_c$), then the phase below threshold would be given by $\langle \phi \rangle = \sin^{-1}[E/E_c] = \sin^{-1}[\theta_c/\pi]$ according to the classical sine-Gordon model (as indicated by the x’ed line in Fig.2). However, when $\tau << 1$, the phase displacements can be much smaller than these classical s-G predictions, right up to the critical value $\theta = \pi$ above which an instanton transition can occur without violating conservation of energy. (Note that $E_T < E_c$ if $\tau << 1$.) The square in Fig. 2 represents the experimental result reported in Ref. [11], which is consistent with our calculations, provided we take the pinning energy $D\omega_0^2$ to be much larger than the electrostatic energy $u_E$ ($\tau \approx 0.02$ in this case). When $D\omega_0^2 >> u_E$ the threshold field for pair creation $E_T$ will be much smaller than the classical pinning field $E_c$. The observed small phase displacements indicated by Refs. [11-14] are all consistent with $E_T$ being small compared to $E_c$.

Figure 3 shows plots of energy density obtained using Eq. (8) vs. $\theta$ for a case where the pinning energy dominates over the electrostatic energy (i.e. for $\tau = 0.2$). From Fig. 3, one can immediately see that the instanton transition is forbidden unless $\theta > \pi$. When the applied electric field is below threshold ($\theta < \pi$), pair creation is prevented by Coulomb blockade. One can gain additional insight into the problem by considering the case when the applied field is equal to its critical value, i.e. $\theta = \pi$. Figure 4 shows plots, obtained from Eqs. (9), of $\langle \phi \rangle$ and the mass ratio $m/m_0$ as functions of the parameter $\tau$ for the case where $\theta = \pi$. Note the bifurcation that occurs when $\tau \approx 0.87$. Thus, more than one metastable state will exist only when $\tau$ is less than this critical value (i.e. when the pinning energy is greater than the electrostatic energy).

The transition temperatures for DW formation can be quite high, well above 200 K in a number of materials. The coupling between parallel DW chains and resulting 3-D coherence must therefore suppress thermal excitations of the S-S' pairs, whose energy would be extremely small if only a single transverse degree of freedom was considered. Ref. [3] provides heuristic scaling arguments on how thermal excitations might be suppressed without suppressing the S-S' tunneling amplitude for an intermediate range of coupling strengths, where the CDW electrons remain delocalized in real space. The situation here may be analogous to Josephson tunneling, where individual Cooper pairs tunnel through an insulating barrier even though the condensed pairs comprise a condensate
with a single thermal degree of freedom. A complete theoretical treatment of DW transport should consider many interacting scalar fields $\phi_n$ and, perhaps, generalize the concept of coherent Josephson-like tunneling. The implications of a collective quantum mechanism of DW depinning are potentially profound and far-reaching, so further work is warranted to experimentally test the predictions here, and to further develop a DW depinning model based on the principles of quantum field theory.

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Fig.1 (a) A materialized soliton-antisoliton pair, showing the position-dependent phase $\phi(x)$, excess charge density $\delta\rho(x) = -(e^*/2\pi) \partial \phi / x$, and internal field $E^* = e^*/\varepsilon A$. (b) The time-evolution of the phase $\phi(x,t)$, illustrating the nucleation and subsequent annihilation of three pairs during the first cycle. Nucleation of additional pairs is blocked in the lightly shaded regions (due to the internal field, -$E^*$) until all pairs have annihilated, thus leading to time-correlated pair creation and annihilation.

Fig.2 $\langle \phi \rangle$ vs. $\theta$ for $\tau = 0.02$ (stars), 0.2 (circles), 0.87 (dashed line), and 1.5 (diamonds). The solid lines through the symbols indicate the lowest energy states. The x’ed line represents the classical sine-Gordon prediction (defining $\theta = \theta_c \equiv \pi E/E_c$), while the square represents the experimental results obtained by Ross et al. [11]

Fig.3 Energy vs. electric field ($\theta$) for $\tau = 0.2$, showing the two branches corresponding to $\langle \phi \rangle \approx 0$ (stars) and $\langle \phi \rangle \approx 2\pi$ (circles).

Fig.4 $\langle \phi \rangle$ vs. $\tau$ (left hand axis, circles), and mass ratio $m/m_0$ vs. $\tau$ (right-hand axis, stars) for $\theta = \pi$. Note that the system bifurcates when $\tau \approx 0.87$. 

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