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QUANTUM DYNAMICS OF CHARGE-DENSITY WAVE SYSTEMS

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In order to derive an effective action which describes low-frequency long-wavelength phenomena in charge-density wave systems, we start from the microscopic model of electrons, coupled to phonons and scattered by impurities, and proceed similar to recent work of Ambegaokar, et. al. The analogy to Josephson junctions, as well as the dissipative contribution to the action are discussed

1. INTRODUCTION

Various models have been proposed to account for the unusual properties of linear-chain compounds, e.g., the nonlinearity of the dc conductivity. Of wide use is the sine-gordon equation for the phase of the order parameter, $\chi(x,t)$ (see below):

$$\ddot{\chi} - c^2 \partial_x^2 \chi + \gamma \dot{\chi} = - U'(\chi) \tag{1}$$

$U(\chi)$ is a tilted periodic potential, $c=v_F/\sqrt{m_F}$, where v_F is the Fermi velocity, $m_F=1+4 \ |\Delta|^2/\lambda\omega_Q^2$, and the damping coefficient γ is expected to be of the order of the single particle scattering rate divided by $m_F (m_F >> 1)$. Data suggest that $\gamma >> \omega_0$, where $\omega_0^2 = U''(0)$. As an extension to classical theories as defined in Eq. 1, it was argued that macroscopic quantum tunneling plays an important role (1,2). Considering the importance of dissipation, a careful investigation of the (quasi-one-dimensional) CDW systems becomes necessary. An interesting aspect is, on the other hand, the formal analogy of Eq. 1 to the RSJ model of Josephson junctions, which suggests that similar methods should be applicable (3,4).

2. MICROSCOPIC THEORY

We start from a microscopic model describing electrons which are coupled to phonons, and scattered by impurities, in the path-integral formulation in "imaginary" time. At the low temperatures under consideration, the quasi-classical theory can be formulated, in terms of the electrons close to the Fermi surface, i.e. in a certain range of momentum near $+p_F$, $-p_F$. (We study one dimension only.) Taking only the phonons with wave vector $\pm Q$, $Q=2p_F$, into account (the commensurable case is discussed below), and "integrating out" the electron variables, we arrive at a partition function/generating functional of the following form:

$$Z = \int D\Delta D\Delta^* \ \exp - S[\Delta,\Delta^*] \tag{2}$$

where $S=S_{ph} + S_{el}$. The phonon part of the action is given by

$$S_{ph} = N(0) \int dxdt \ \Delta^* D_o^{-1} \Delta/\lambda$$
$$D_o^{-1} = 1 - \omega_Q^{-2} \partial_t^2 \tag{3}$$

with $N(0) = 1/\pi v_F$, $\lambda = N(0)g^2$. Magnitude and phase of the order parameter are introduced via $i\Delta = |\Delta| \exp(-i\chi)$. The electron part of the action is given by

$$S_{el} = - \text{tr} \log \hat{G}^{-1} \tag{4}$$

where $\hat{G}^{-1}$ is a 2 x 2 matrix labelled by $\pm p_F$. We write

$$\hat{G}^{-1} = Q_\alpha \ \hat{\tau}_\alpha \ \delta(x-x') \ \delta(t-t') \tag{5}$$

$\hat{\tau}_\alpha$, $\alpha = 1,2,3$, are the Pauli matrices; $\hat{\tau}_o=\hat{1}$. The result is

$$Q_o = \frac{i}{2}(\partial_t\chi) + ev_F A + iv_F\partial_x$$
$$Q_3 = - \partial_t + \frac{1}{2} v_F(\partial_x\chi) - e\varphi - \eta$$
$$Q_1 = i\{|\Delta| + \text{Im}(\xi \exp i\chi)\} \tag{6}$$
$$Q_2 = i \ \text{Re}(\xi \exp i\chi)$$

The stochastic field $\eta(x)$, $\xi(x)$, the latter being complex, describe impurity scattering, and have a Gaussian distribution with

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$$\langle\eta\rangle_i = \langle\xi\rangle_i = \langle\eta\xi\rangle_i = \langle\xi\xi\rangle_i = 0$$
$$\langle\eta(x)\eta(x')\rangle_i = \delta(x-x')\ v_F/2\tau_1 \qquad (7)$$
$$\langle\xi(x)\xi^*(x')\rangle_i = \delta(x-x')\ v_F/2\tau_2$$

Here, $\tau_1(\tau_2)$ are the scattering times for $p_F \leftrightarrow +(-)p_F$, respectively. The scattering rates are related to the pair-breaking parameter Γ, often introduced in superconductivity, by

$$\Gamma = (2\tau_1)^{-1} + (4\tau_2)^{-1} \qquad (8)$$

Finally, A and φ are the electromagnetic fields.

In contrast to Eq. 5, the description of a Josephson junction (4) leads to a 4 x 4 matrix Green's function, with the consequence that, in the limit of the transfer matrix element going to zero, the two superconductors are decoupled, and the electron charge is conserved individually. An analogous statement, for $\xi \to 0$, cannot be made here.

3. COMMENSURABLE CDW SYSTEMS

Commensurable situations can be easily included in the present formalism. Then, for some integer N, we have $NQ=2\pi/a$, where a is the lattice constant. In general, additional phonons have to be included, and Eq. 5 has to be replaced by a N x N matrix. For example, for N=3, the complex field Δ, as introduced above, is sufficient, while for N=4, an additional (real) field is needed. However, since the Fermi energy is much larger than all energies of interest, the phase dependent part of the action can be calculated easily.

4. RESULTS

We proceed from Eq. 2 and expand the action with respect to slow variations in space and time, and with respect to the electromagnetic and impurity fields. Commensurability effects with N=3,4 are included. Also, we restrict ourselves to zero temperature, and ignore variations of, and consider the stationary point with respect to, the magnitude of the order parameter (and with respect to the additional phonon field, for N=4). Variations of $|\Delta|$ are expected to become important only for high frequencies, of the order ω_Q. We arrive at an effective action, S_{eff}, which we write as

$$S_{eff}[\chi] = S_o + S_1 + S_2 \qquad (9)$$

S_o corresponds to the non-dissipative part of Eq. 1, and we obtain the standard result. Corrections to the commensurability potential were obtained, and turn out to be $\sim\omega_Q^{-2}(\partial_t\chi)^2$. The diagonal impurity field, η, can be included by the replacement $e\varepsilon \to e\varepsilon - \partial_x\eta$, where ε is the electric field. The remaining terms in the action S_1 and S_2, are linear and quadratic in ξ, respectively. We find

$$S_1 = \rho_1 \int dxdt\ \mathrm{Re}(i\xi\ \exp i\chi) \qquad (10)$$

where ρ_1 is the CDW amplitude, $\rho_1=2|\Delta|/g^2$. This is the "classical" (3) impurity pinning. In S_2, we find additional terms contributing to pinning, of the form

$$\xi(x)\xi(x')\ \exp i\{\chi(x,t) + \chi(x',t')\} \qquad (11)$$

see Ref. (3) and others related to dissipation, as discussed below:

$$\xi(x)\xi^*(x')\ \exp i\{\chi(x,t) - \chi(x',t')\} \qquad (12)$$

Taking the impurity average of S_2, upon which terms as in Eq. 11 vanish, we obtain

$$\langle S_2\rangle_i = \frac{m_F}{\pi v_F}\int dxdtdt'$$
$$\times\ \alpha(t-t')\ \sin^2\{\frac{\chi(x,t)-\chi(x,t')}{2}\} \qquad (13)$$

where $\alpha(t)$ is given by $(\gamma = (m_F\tau_2)^{-1})$

$$\alpha(t) = \frac{\gamma}{2\pi}\ \{|\Delta|\ K_1(|\Delta|t)\}^2 \qquad (14)$$

and reduces to the function defined in (2) for $|\Delta| \to 0$. In this limit, the analytic continuation to real times of the impurity averaged action shows that the action is equivalent to Eq. 1, however, with a noise term of the shot noise type, depending on the bias current. For $|\Delta| \neq 0$, $\alpha(t)$ decreases exponentially for large t, reflecting the gap in the excitation spectrum. In this case, Eq. 13 can be interpreted as a (very small) correction to the effective mass (4). Details of our calculation as well as further discussions of the results, will be published elsewhere.

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