Numerical Study of Collective Transport in Charge Density Wave Conductors

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Abstract. We present the results of numerical simulation of the sliding conduction of charge density wave using newly derived time-dependent equations of motion of the Ginzburg-Landau type. In this analysis, the quasi-particle fluctuation modes are treated as independent variables and electron injection to and extraction from the charge density wave conductor are directly simulated.

1. Introduction
The intriguing conduction phenomena in charge density waves (CDW’s) have long been studied by various people and many effective concepts have been developed, including dislocation-mediated phase slip \cite{1, 2, 3}. It has been recognized that the dynamics of dislocations in charge density waves is largely affected by the quasi-particle dynamics in the conductors. Especially, electron conversion between condensate and quasi-particle sub-systems at the cores of moving dislocations has been discussed, which is sometimes called “spectral flow” phenomena \cite{4, 5}.

Several numerical studies in order to clarify the sliding conduction of CDW has been done based on the time-dependent Ginzburg-Landau (GL) theory \cite{6, 7}. Since GL equation is obtained after integrating out the quasi-particle degree of freedom, the motions of quasi-particles cannot be treated in a direct way. Moreover, the non-equilibrium nature of quasi-particle sub-system may be underestimated within such a framework.

We have recently developed a new set of time-dependent equations, which enables us to study quasi-particle dynamics in more direct and apparent way \cite{8}. In this paper we present the results of numerical simulations based on our equations.

2. Model equations
We consider the one-dimensional CDW conductor with two current electrodes. The equations of motion of the CDW order parameter, $\Delta(x, t)$, and the chemical potential of right-moving and left-moving electrons, $\mu_R(x, t)$ and $\mu_L(x, t)$, are introduced as follows. First we define the sum and the difference of two chemical potentials, $\mu_s = \mu_R + \mu_L$, $\mu_a = \mu_R - \mu_L$, and, then, the charge...
density $\rho = \rho_q + \rho_c$ and the current $j = j_q + j_c$ of the system are given as

$$\rho_q = -\frac{e}{2\pi \hbar v_F} \left( 1 - \frac{c_1}{T^2} |\Delta|^2 \right) \mu_s, \quad \rho_c = i \frac{ec_1}{4\pi T^2} \left( \Delta^* \partial_x \Delta - \partial_x \Delta^* \Delta \right),$$

(1)

$$j_q = -\frac{e}{2\pi \hbar} \left( 1 - \frac{c_1}{T^2} |\Delta|^2 \right) \mu_a, \quad j_c = -i \frac{ec_1}{4\pi T^2} \left( \Delta^* \partial_t \Delta - \partial_t \Delta^* \Delta \right),$$

(2)

where quantities with suffixes “q” and “c” are the contributions of quasi-particles and condensate, respectively. Here $e$, $v_F$ and $T$ are electron charge, Fermi velocity and temperature, respectively. $c_1 = \frac{7\zeta(3)}{4\pi^2}$ with $\zeta(z)$ being zeta function. The condensate obeys the following GL-type equation,

$$\hbar \partial_t \Delta + i \mu_a \Delta = \frac{8T_c}{\pi} \left( 1 - \frac{T}{T_c} \right) \Delta + \frac{8c_1}{\pi T_c} \left( \left( \frac{hv_F}{\mu_s} \right)^2 \left( \partial_x - \frac{i \mu_s}{hv_F} \right)^2 \Delta - \frac{|\Delta|^2 \Delta}{2} \right) + \alpha(x),$$

(3)

where $T_c$ is the critical temperature. A complex function $\alpha(x)$ is introduced to incorporate the effects of pinning. For example, if we take $\alpha$ to be real and positive, $\Delta$ is stabilized on the positive real axis. The motion of quasiparticle is governed by Boltzmann-type equation,

$$\frac{\hbar}{e} \partial_t j + \frac{(hv_F)^2}{e} \partial_x \rho - \frac{hv_F E}{\pi} = \frac{\hbar}{2\pi \tau_{tr}} \left( 1 - \frac{2c_1}{T^2} |\Delta|^2 \right) \mu_a,$$

(4)

where $\tau_{tr}$ is the transport life time of quasiparticles. In the actual numerical simulation, the first term of Eq. (4) is neglected for simplicity. The full Ginzburg-Landau equation is complimented with the Gauss’ law, $\partial_x E = 4\pi \rho / S$ and the charge conservation law, $\partial_t \rho + \partial_x j = \Gamma$, where $S$ is the effective cross section of the chain and $\Gamma(x,t)$ is the externally supplied current source. By solving these equations together under an apropriate initial condition, the parameters describing the system, $\Delta$, $\mu_s$, $\mu_a$, and $E$, are determined. The microscopic basis of these equations will be discussed elsewhere [8].

### 3. Geometry of the Simulation

In this paper we consider two configurations of the system. The CDW conductor (length $L$) is assumed to be pinned near the both ends. We set $x$-axis along the CDW ($0 \leq x \leq L$). The electrodes, at which electric current is injected and extracted, are located respectively at $x = x_i$ and $x = x'_i$. CDW is assumed to be pinned in the regions, $0 \leq x \leq x_p$ and $x'_p \leq x \leq L$. In this calculation, for simplicity, we set $\alpha(x)$ to be a real and positive constant in these regions.

![Figure 1](image-url) **Figure 1.** Two configurations of the simulation: current electrodes are located in the regions where (a) CDW is not pinned, and (b) CDW is pinned.
4. Numerical Results

There are several parameters important for the simulation. The value of $\Delta$ is normalized by its equilibrium value at $T = 0$, namely $\Delta_0 = k_B T_c \sqrt{2} c_1$. Time is normalized by the relaxation time of the condensate, $\tau = \hbar/8T_c$ and the length by the CDW coherence length at $T = 0$, $\xi_0 = h v_F \sqrt{\tau}/(2 k_B T_c)$. The electron number density $\rho_e$ in the equilibrium, the electrostatic screening length $\lambda$ and the conductivity $\sigma$ are given respectively by $\rho_e = n v_F/(\pi \hbar)$, $\lambda^{-2} = 4 e^2/(h v_F S)$ and $\sigma = \tau_\text{rel} n \rho_e / m$, where $m$ is the electron mass. We also introduce characteristic length, $l = v_F \tau_\text{rel}$, and $l_c = v_F \tau$, where the former is the usual mean free path of the electrons.

In the following numerical results, the parameters are taken as follows, $L = 50 \xi_0$, $T = 0.95 T_c$, $l c / (\pi \xi_0^2) = 0.1$. The equilibrium value of $\Delta$ is $0.815 \times \Delta_0$ in the pinned regions and $0.224 \times \Delta_0$ in the pin-free region. (Since rather strong pinning is introduced in this calculation, $\Delta$ is much enhanced in the pinned regions.)

Here we note that a divergent contribution can arise in our framework when $|\Delta|$ becomes large. It comes from the factors such as $(1 - c_1|\Delta|^2 / T^2)$ appearing in Eqs. (1), (2) and (4), which vanish for large $|\Delta|$. In order to avoid this, we replaced them with non-vanishing forms, e.g. exp$(-c_1|\Delta|^2 / T^2)$.

In fig. 2 we have shown the behavior of $\Delta$ in the configuration shown in fig. 1(a). The current is switched on at $t = 0$ and the graph shows the time evolution up to $T = 60 \tau$. The strength of the current is set as $\xi_0 \tau T = 10.0$. The initial value of $\Delta$ is set to $0.815 \times \Delta_0$ in pinned region and $0.224 \times \Delta_0$ in pin-free region. The position of the current electrodes are $x_i = (2/7)L$ and $x_i' = (5/7)L$, shown by dashed-dotted lines. The boundary of pinned and pin-free region is $x_p = (1/7)L$ and $x_p' = (6/7)L$, shown by dashed lines. One can see the periodic suppression of $\Delta$ in the regions, $x_p < x < x_i$ and $x_p' < x < x_i'$, which is interpreted as the manifestation of dislocation mediated phase slips. It is interesting that the position of the phase slip center is outside of the current electrodes. This, we think, is a new insight provided for the first time by our analysis.

In fig. 3 we have shown the results for the configuration in fig. 1 (b). We set $x_i = (1/7)L$, $x_i' = (6/7)L$, $x_p = (2/7)L$ and $x_p' = (5/7)L$. In contrast to the previous result one can see that $\Delta$ is suppressed at the positions of electron injection and extraction, $x = x_i$ and $x = x_i'$. At these points CDW is completely pinned and there is no condensate current. The quasi-particles are accumulated to generate electric field and, therefore, CDW order is suppressed. One can also see that periodic suppression of $\Delta$ appears near $x_p$ and $x_p'$. These originate from the phase slips, which enable sliding motion of the condensate in pin-free region.

5. Discussion

We have studied the dynamics of CDW conductor under a transport current within a new theoretical framework. One advantage of our frame work is that we can simulate the dynamics of CDW conductors directly with taking account of the non-equilibrium nature of the quasi-particles. Although our results are not very comprehensive at this stage, we consider that several new features have already been revealed. For example, we have shown that the phase slip of CDW can differ between the configuration of the electrodes and pinning potential; as one can see from fig. 2, the phase slips can take place even outside of the current electrodes, when CDW is not pinned near the electrodes. Such a result has not been obtained in the preceding studies.

Although our study is purely one-dimensional at this stage, it is also easy to extend the present framework to three dimension by introducing quasi-particle hopping between chains. In that case, we may be able to treat more complicated phenomena of CDW conduction. We leave this for the further studies.
Figure 2. The behavior of $\Delta$ obtained by numerical solution of our time-dependent equations in the geometry given in fig. 1 (a). We have shown (a) the surface plot of $|\Delta|$ as a function of $x$ and $t$, and (b) the corresponding contour plot.

Figure 3. The numerical results corresponding to fig. 1 (b). (a) and (b) are the same with fig. 2.

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