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# Non-quasiparticle corrections for a sliding charge-density wave

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**Abstract.** The state of the electrons in a charge-density wave (CDW) sliding at arbitrary velocity and with arbitrary electron–phonon coupling constant is discussed. The mean-field framework deals directly with the quantum mechanics of a system having non-energy-eigenstate solutions. The quasiparticle approximation is replaced by a more accurate electron–hole condensate. Corrections to the uniform current, which become important at moderate electron–phonon coupling or at high CDW speed, show that the Fermi sea is swept along with a velocity slightly less than the velocity of the CDW. Corrections to the effective energy gap for photon absorption are also discussed.

## 1. Introduction

The dynamics of a charge-density wave (CDW) in a quasi-one-dimensional conductor has been widely studied [1–13] (see Grüner [10] for a review). As the CDW slides over the lattice, the electrons comprising the wave experience a time-dependent interaction. This time dependence introduces a subtlety in the electron wave functions which has not been properly taken into account so far in the literature. To 'paraphrase' the quantum mechanics occurring here, the wave function for a single electron near the Fermi surface interacting via lattice vibrations with a hole state on the other side of the Fermi surface takes the form

$$|\psi(t)\rangle = a\mathrm{e}^{-\mathrm{i}E_a t}|k_1\rangle + b\mathrm{e}^{-\mathrm{i}E_b t}|k_2\rangle. \tag{1}$$

The interesting fact here is that, e.g.,

$$|\phi(t)\rangle = c\mathrm{e}^{-\mathrm{i}E_a t}|k_1\rangle \tag{2}$$

alone is not a solution of the Schrödinger equation for the electron. Due to the time dependence in the interaction, only wave functions of the form (1) are valid. One could call wave functions of the form (2) quasiparticle solutions. For weak coupling ($g \ll E_F$), the errors incurred in treating quasiparticles as actual solutions are not significant. However, at larger coupling the errors mount. For the electron–phonon coupling typically encountered in sliding CDW systems, the corrections to the uniform current turn out to be about 0.1% at low CDW velocities, and somewhat more at higher velocities.

It is the purpose of the first part of this paper to derive a solution analogous to equation (1), but for a whole band of electrons, then to find the uniform current corresponding to it. In a similar way the time-dependent interaction modifies the effective photon absorption spectrum. This is discussed in the second part of the paper.

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The theory is a mean-field one set up for zero temperature. The focus is on the electrons as they interact with a time-dependent potential formed by a moving periodic lattice distortion (PLD). A similar Hamiltonian has been considered by Horovitz [8]. The motion of the CDW and the accompanying PLD are assumed to result from some previous external field, similarly to how currents in a superconductor might be set up. There is no dissipation, so this field is not included in the Hamiltonian describing the electrons.

The model is introduced in section 2. The spectrum and the solution having the lowest average energy are derived in section 3. The uniform current for this solution is found in section 4. The energy gap and photon absorption are discussed in section 5.

## 2. The model

In order to focus on the central feature the theory will be pared to the bone. Electron–electron interactions, pinning, dissipation, and other thermal effects are omitted. The theory applies to a single electron band, not too full and not too empty, taken to be about half-full so that each electron state can be paired with a hole state.

Consider first the general Hamiltonian

$$H_{gen} = \sum_k \varepsilon_k c_k^+ c_k + \sum_q \omega_q b_q^+ b_q + \sum_{k,q} g_{kq} c_{k+q}^+ c_k (b_q + b_{-q}^+). \tag{3}$$

Here the $c$s are electron operators, the $b$s are phonon operators, and $g_{kq}$ is the electron–phonon coupling constant. The sum over wave vectors $k$ is meant to imply also a sum over electron spin.

Next, narrow attention to a state with a travelling phonon wave at wave vector $q = Q = 2k_F$ described by an order parameter

$$g\mathrm{e}^{\mathrm{i}\omega t} = g_{k_F Q}\langle b_Q + b_{-Q}^+\rangle. \tag{4}$$

In real space this corresponds to a phonon wave with an amplitude $\langle y\rangle$ at position $x$ of

$$\langle y\rangle \sim \cos(Qx + \omega t). \tag{5}$$

The mean-field Hamiltonian for the electrons in this phonon wind is

$$H = \sum_k \varepsilon_k c_k^+ c_k + g\sum_k [\mathrm{e}^{\mathrm{i}\omega t} c_{k+Q}^+ c_k + \mathrm{e}^{-\mathrm{i}\omega t} c_k^+ c_{k+Q}]. \tag{6}$$

The sum over $k$ will be restricted to $-2k_F < k < 0$. This simplification causes each relevant $k$-state to be paired with just one other state. This is a good approximation since the difference in energy between interacting states is lowest for these pairings. Since the calculation is done at zero temperature, all electron states in the band are paired to make the CDW condensate.

## 3. The spectrum and solution

A typical pair of terms in $H$ is (see figure 1)

$$H_1 = \varepsilon_1 c_1^+ c_1 + \varepsilon_2 c_2^+ c_2 + [g\mathrm{e}^{\mathrm{i}\omega t} c_1^+ c_2 + \mathrm{h.c.}]. \tag{7}$$

Let $|\psi\rangle$ represent a state of the electron evolving under Hamiltonian $H_1$. Solving $H_1|\psi\rangle = E|\psi\rangle$ gives the energy eigenvalues

$$E_\pm = \frac{(\varepsilon_1 + \varepsilon_2)}{2} \pm \sqrt{g^2 + \frac{(\varepsilon_1 - \varepsilon_2)^2}{4}}. \tag{8}$$

Upon measurement of the electron's energy, of course one of the two values will be obtained. This is well accepted (see, e.g., reference [14]). This gives the spectrum shown in figure 2. Note that there is no dependence on $\omega$, i.e. on the velocity $V$ of the wave ($V = \omega/Q$).

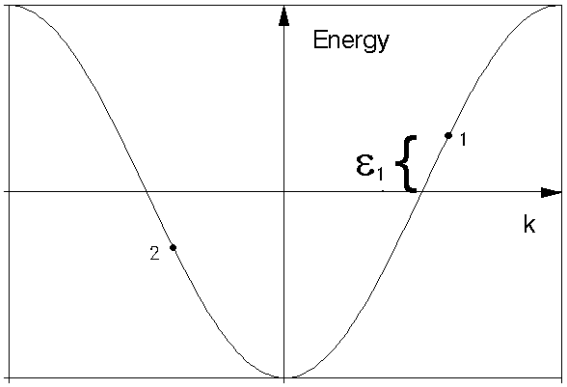


**Figure 1.** The band structure showing a pair of interacting states.

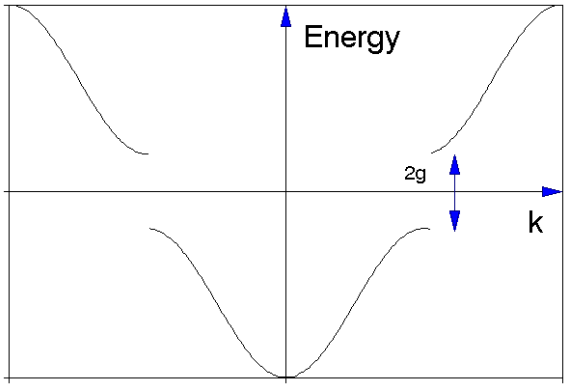


**Figure 2.** The spectrum of $H$.

At this stage one could make a time-dependent gauge transformation and find the quasiparticle spectrum (see Bjelis [9]). However, it is important to realize that there is an error made in treating the electron as a quasiparticle with definite energy. It is the goal of the present work to avoid this error, and see what corrections ensue. Here the electron states are treated accurately in pairs, then summed to give the band result. As a price to pay, the expression for the uniform current has a less classical form, and the effective energy gap becomes process dependent.

First the solution to

$$\mathrm{i}\frac{\mathrm{d}|\psi\rangle}{\mathrm{d}t} = H_1|\psi\rangle \tag{9}$$

is found (Planck's constant is temporarily set equal to $2\pi$). The solution is written as

$$|\psi\rangle = a_1(t)|1\rangle + a_2(t)|2\rangle \tag{10}$$

where

$$|1\rangle = c_1^+|0\rangle \qquad |2\rangle = c_2^+|0\rangle \tag{11}$$

and $|0\rangle$ is the no-particle state. One finds

$$a_1 = \gamma_1 \mathrm{e}^{\mathrm{i}\alpha_1 t} + \gamma_2 \mathrm{e}^{\mathrm{i}\alpha_2 t} \tag{12}$$

$$a_2 = -g^{-1}\mathrm{e}^{-\mathrm{i}\omega t}[\gamma_1(\varepsilon_1 + \alpha_1)\mathrm{e}^{\mathrm{i}\alpha_1 t} + \gamma_2(\varepsilon_1 + \alpha_2)\mathrm{e}^{\mathrm{i}\alpha_2 t}] \tag{13}$$

where

$$\alpha_1 = \frac{1}{2}[\omega - (\varepsilon_1 + \varepsilon_2) + \sqrt{4g^2 + (\varepsilon_1 - \varepsilon_2 + \omega)^2}] \tag{14}$$

$$\alpha_2 = \frac{1}{2}[\omega - (\varepsilon_1 + \varepsilon_2) - \sqrt{4g^2 + (\varepsilon_1 - \varepsilon_2 + \omega)^2}]. \tag{15}$$

$\gamma_1$ and $\gamma_2$ are arbitrary, subject to the normalization condition

$$1 = [1 + g^{-2}(\varepsilon_1 + \alpha_1)^2]|\gamma_1|^2 + [1 + g^{-2}(\varepsilon_1 + \alpha_2)^2]|\gamma_2|^2. \tag{16}$$

Evaluating the expectation value of $H_1$ for a solution yields

$$\langle H_1 \rangle = \langle H_1 \rangle_{t-\text{dep}} + \langle H_1 \rangle_{t-\text{indep}} \tag{17}$$

where

$$\langle H_1 \rangle_{t-\text{dep}} = (-1)(\varepsilon_1 + \varepsilon_2 + \alpha_1 + \alpha_2)(\gamma_1 \gamma_2^* \mathrm{e}^{\mathrm{i}(\alpha_1 - \alpha_2)t} + \text{c.c.}) \tag{18}$$

$$\langle H_1 \rangle_{t-\text{indep}} = |\gamma_1|^2[\varepsilon_1 - 2(\varepsilon_1 + \alpha_1) + g^{-2}\varepsilon_2(\varepsilon_1 + \alpha_1)^2] + |\gamma_2|^2[\varepsilon_1 - 2(\varepsilon_1 + \alpha_2) + g^{-2}\varepsilon_2(\varepsilon_1 + \alpha_2)^2]. \tag{19}$$

The solution with the lowest time-averaged energy has $\gamma_2 = 0$, with no time-dependent part. For simplicity, measure energies from the Fermi level, and specialize to the case where $\varepsilon_1 = -\varepsilon_2$ ($=\varepsilon$, say). Then the expectation value of $H_1$ for this state of lowest average energy (call it the ground state) is evaluated as

$$\langle H_1 \rangle_{ground} = -\frac{2g^2 + \varepsilon(2\varepsilon + \omega)}{\sqrt{4g^2 + (2\varepsilon + \omega)^2}} \qquad \text{(type 1 pairing)}. \tag{20}$$

Carrying out a similar analysis for a pairing of states with the positive-momentum state being below the Fermi surface (type 2 pairing), one finds

$$\langle H_1 \rangle_{ground} = -\frac{2g^2 + \varepsilon(2\varepsilon - \omega)}{\sqrt{4g^2 + (2\varepsilon - \omega)^2}} \qquad \text{(type 2 pairing)}. \tag{21}$$

Figure 3 shows the average energies of ground-state pairs as well as the average energies of the sky state (largest-energy) pairs.

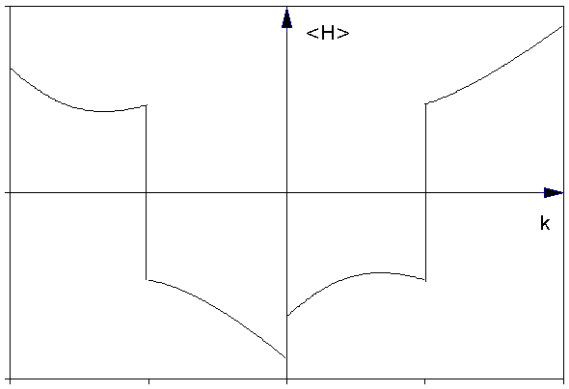


**Figure 3.** The range of average energies for solutions.

Let us review this section. Equation (8) (the spectrum) gives the two possible results arising from a measurement of the electron's energy. One might be tempted to find the solutions corresponding to each one of these energies. But such solutions do not exist. The time

dependence in the interaction causes the solutions not to have a definite energy, but instead to have only an amplitude for having each of the spectral energies. This solution is now kept intact for each of the electrons in the band while the physical properties of the band are calculated.

## 4. The current

Consider simultaneously a pair of states (1, 2) with type 1 pairing and a pair (3, 4) with type 2 pairing, with members of a pair above and below the Fermi level by an energy $\varepsilon$. Approximating the states as being free with an effective mass $m$, and linearizing about the Fermi level ($k_1 = k_F + \delta, k_2 = -k_F + \delta, k_3 = -k_F - \delta, k_4 = k_F - \delta$), then the 0 and $Q$ Fourier components of the current density are given by

$$\langle j_0 \rangle_{2\,pairs} = \frac{Q_e k_F}{m}[\langle c_1^+ c_1 \rangle - \langle c_2^+ c_2 \rangle + \langle c_4^+ c_4 \rangle - \langle c_3^+ c_3 \rangle] \tag{22}$$

$$\langle j_Q \rangle_{2\,pairs} = \frac{Q_e \delta}{m}[\langle c_1^+ c_2 \rangle - \langle c_4^+ c_3 \rangle]. \tag{23}$$

Here $Q_e$ is the charge on the electron. The Fourier components of the total current can now be evaluated. In particular,

$$\langle j_0 \rangle_{total} = 2N(0) \int_0^{E_c} \langle j_0 \rangle_{2\,pairs}\, \mathrm{d}\varepsilon. \tag{24}$$

Here $2N(0)$ is the density of electron states at the Fermi level including spin, and $E_c$ is the cut-off energy corresponding to the bandwidth.

Evaluation of equation (22) for the ground state yields

$$\langle j_0 \rangle_{2\,pairs} = \frac{Q_e k_F}{m}\left[\frac{g^2 - (\varepsilon + \alpha_1)^2}{g^2 + (\varepsilon + \alpha_1)^2} - \frac{g^2 - (\varepsilon + \alpha_3)^2}{g^2 + (\varepsilon + \alpha_3)^2}\right] \tag{25}$$

where $\alpha_3$ is just $\alpha_1$ with $\omega$ replaced by $-\omega$. Integrating (24) yields

$$\langle j_0 \rangle = -\frac{N(0) Q_e k_F}{m}\left[\sqrt{4g^2 + (2E_c + \omega)^2} - \sqrt{4g^2 + (2E_c - \omega)^2}\right]. \tag{26}$$

In the limit of low CDW velocity ($\omega \ll g$), equation (26) becomes

$$\langle j_0 \rangle = -\left(\frac{2N(0) Q_e k_F}{m}\right)\left(\frac{E_c \omega}{\sqrt{E_c^2 + g^2}}\right)\left(1 - \frac{1}{8}\frac{g^2 \omega^2}{(E_c^2 + g^2)^2}\right). \tag{27}$$

For the parabolic band assumed here, $E_c = \hbar^2 k_F^2 / m$, so upon introducing the necessary factors to express all quantities in conventional (SI) units, i.e. $g_{con} = \hbar g$, $j_{con} = \hbar^2 j$, the expression for the total uniform current becomes

$$\langle j_0 \rangle = -2\left(\frac{N(0) Q_e}{k_F}\right)\left(\frac{E_c^2 \omega}{\sqrt{E_c^2 + g^2}}\right)\left(1 - \frac{1}{8}\frac{g^2 \hbar^2 \omega^2}{(E_c^2 + g^2)^2}\right). \tag{28}$$

On the other hand, for two electrons to be merely swept along at the same speed as the CDW one would have $\langle j_0 \rangle = \rho_0 V$, which with $V = \omega/(2k_F)$ would read

$$\langle j_0 \rangle_{2\,pairs,\,swept\,along} = -(2Q_e)\left(\frac{\omega}{2k_F}\right) \tag{29}$$

so this uniform current would be

$$\langle j_0 \rangle_{total,\,swept\,along} = -2N(0) E_c Q_e \left(\frac{\omega}{k_F}\right). \tag{30}$$

For comparison purposes, the actual uniform current can be written as

$$\langle j_0 \rangle = \langle j_0 \rangle_{swept\ along} \left( \frac{E_c}{\sqrt{E_c^2 + g^2}} \right) \left( 1 - \left( \frac{g^2}{E_c^2} \right) \left( \frac{\frac{1}{2} m V^2}{E_c} \right) \right). \tag{31}$$

This form illustrates separately the corrections due to stronger coupling and to high CDW velocities.

The usual quasiparticle picture has $\langle j_0 \rangle = \langle j_0 \rangle_{swept\ along}$. This comes from writing the uniform current as

$$\langle j_0 \rangle = 2 Q_e \int \left( \frac{\mathrm{d}E}{\mathrm{d}k} \right) \mathrm{d}k \tag{32}$$

and using a band structure modified by the sliding CDW (see, e.g., reference [10]). The error enters upon assuming that the (quasi)particles have a definite energy. In contrast, here the condensate consists of electrons each having an amplitude for being in two different energy eigenstates.

To clarify the above picture it is useful to consider the opposite case of strong coupling ($g \gg E_c$). At large coupling all pairs of electron states $|+k\rangle$ and $|-k\rangle$ would be occupied with almost the same probability, namely 1/2. Physically, the electrons are being strongly scattered by the ions. Nearly equal occupation of electron states of opposite momentum means that the uniform current will be small. However, the velocity of the sliding CDW can still be large. This is like ripples on a pond, where the ripples can be moving along at any speed while the body of water below can be still, giving a small uniform current.

The corrections to be expected can be estimated for a typical weakly coupled system. Following Grüner [10], the coupling constant $g$ can be written as $g^2 = \lambda(\hbar\omega^0)E_F$, where $\lambda$ is the dimensionless electron–phonon coupling constant, and $\omega^0$ is the phonon frequency at wave vector $2k_F$. $\lambda$ can in turn be related to the Peierls transition temperature $T_P$ through the BCS equation for the energy gap and the relation $\Delta = 1.76\, k_B T_P$. This yields

$$\frac{g^2}{E_c^2} = \frac{(\hbar\omega^0)E_F}{E_c^2 \log(4E_c/\Delta)}. \tag{33}$$

Evaluating this expression for the well-studied compound $NbSe_3$, with $E_c \approx 1$ eV, $E_F \approx 1$ eV, $\Delta \approx 10^{-2}$ eV, $\hbar\omega^0 \approx 10^{-2}$ eV, gives $(g/E_c)^2 \approx 0.0017$. Using this value in equation (31), the actual low-velocity current is lower than the swept-along prediction by about 0.1%. Only at velocities sizable compared to the Fermi velocity is the velocity correction factor important. How robust is this result? The linear band approximation could result in a changed effective energy cut-off. But all states are connected by a single wave vector, so, e.g., wave-vector dependence of the coupling constant will not be important.

In a given experimental situation there may be other effects clouding the picture, such as finite temperatures and impurities. However, the effects of non-zero electron–phonon coupling and non-zero velocity in a sliding wave are present in all sliding CDW systems—hence the attention paid to them here.

## 5. The energy gap and photon absorption

For a CDW sliding with any non-zero velocity, technically there is no energy gap. This shows up in the present analysis in the fact that one can continuously vary the coefficients $\gamma_1$, $\gamma_2$ and arrive at solutions with average energies ranging from the ground-state energy continuously upward. However, in an experimental setting the question is which excitations can produce these intermediate states.

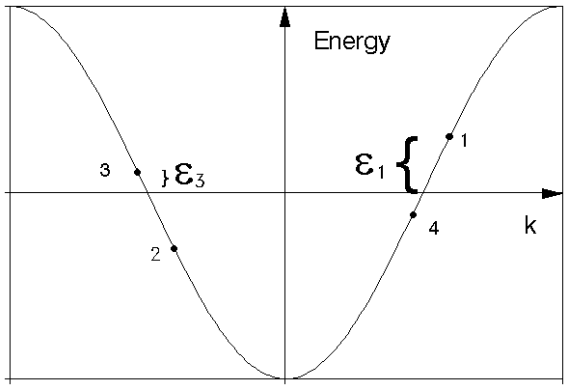


**Figure 4.** Four states involved in photon absorption.

Regarding photon absorption, there is an effective gap, since electron states of given momentum difference must be separated by a large energy. The goal here is to find the basic effect that the sliding CDW has on photon absorption. Spin and three-dimensional considerations are omitted.

Absorption of a photon requires a relatively small momentum for the energy involved, so, e.g., electron states 1 and 4 in figure 4 below might be relevant. But since interaction with the phonons couples these electron states to states 2 and 3, absorption of a single photon actually involves four electron states.

After interaction with the lattice, the electron state formed from states 1 and 2 is not an energy eigenstate, and similarly for the state formed from 3 and 4. So it is not quite correct to merely consider photon absorption across the Peierls gap, as determined by, say, the average of the Hamiltonian, $\langle H \rangle$. Given the above set of four states 1, 2, 3, 4, characterized by energies $\varepsilon_1$ and $\varepsilon_3$, the following procedure leads to the photon frequency absorbed by the set of states.

Using the number representation, $|n_1, n_2, n_3, n_4, n_{photon}\rangle$, the state (including a photon of frequency $\nu$) before photon absorption is

$$|\Psi_i\rangle = \mathrm{e}^{-\mathrm{i}\nu t}\{f_{13}|10101\rangle + f_{14}|10011\rangle + f_{23}|01101\rangle + f_{24}|01011\rangle\}. \tag{34}$$

Here $f_{13}(t) = a_1(t)a_3(t)$, etc.

The interaction can be taken to be

$$H'_{1234} = ha(c_1^\dagger c_4 + c_2^\dagger c_3) + \text{h.c.} \tag{35}$$

where $a$ is a photon destruction operator for a photon with momentum $k_1 - k_4$ $(=k_2 - k_3)$ and $h$ is the strength of interaction. In general, the state of the two electrons and one photon can be written as

$$|\Psi_{all}(t)\rangle = \lambda_i(t)|\Psi_i(t)\rangle + \lambda_f(t)|\Psi_f\rangle \tag{36}$$

with $\lambda_i(0) = 1$, $\lambda_f(0) = 0$ and $|\Psi_f\rangle = |11000\rangle$. Then one has

$$H'_{1234}|\Psi_i(t)\rangle = h\mathrm{e}^{-\mathrm{i}\nu t}(f_{13} + f_{24})|11000\rangle. \tag{37}$$

Evaluation of $f_{13} + f_{24}$ yields

$$f_{13} + f_{24} + [1 + g^{-2}(\varepsilon_1 + \alpha_1)(\varepsilon_3 + \alpha_3)]\gamma_1\gamma_3\mathrm{e}^{\mathrm{i}(\alpha_1+\alpha_3)t}. \tag{38}$$

Following a procedure like that for deriving Fermi's Golden Rule (see, e.g., reference [15]), the transition probability rate $P$ is found to be

$$P = 4\pi|h|^2|\gamma_1|^2|\gamma_3|^2[1 + g^{-2}(\varepsilon_1 + \alpha_1)(\varepsilon_3 + \alpha_3)]^2\delta(\nu - \alpha_1 - \alpha_3). \tag{39}$$

The important fact here is that the photon absorption peaks at a frequency of $\nu = \alpha_1 + \alpha_3$, i.e. at a frequency of

$$\nu = (1/2)[\sqrt{(4g^2 + (2\varepsilon_1 + \omega)^2)} + \sqrt{(4g^2 + (2\varepsilon_3 - \omega)^2)}]. \tag{40}$$

Thus the effective band structure appropriate to photon absorption is

$$E_{photon\,absorption} = \sqrt{(g^2 + (\varepsilon + \omega/2)^2)} \tag{41}$$

written in terms of the non-interacting band energy $\varepsilon = v(k - k_F)$. Comparison with equation (20) shows that whereas the average energy gap decreases with increasing CDW velocity for states near the gap, the energy gap relevant to photon absorption increases with increasing CDW velocity for these same states.

## 6. Conclusions

The focus has been on what an electron experiences while being part of a sliding CDW. Conceptually, the difference between the usual viewpoint and the one espoused here is large. In the usual view, quasiparticles are imagined to be in definite energy states. An increase in the uniform current arises from new states being occupied. However, the particles are not really in definite energy states. In the new picture the notion of a condensate consisting of electrons each having an amplitude for being in each of two energy eigenstates is embraced. An increase in current arises from an increased amplitude for being in the upper energy state.

For a typical sliding CDW, the numerical differences between the two approaches are small. This arises, as seen in equation (33), mainly due to the small phonon energy compared to the electron bandwidth.

The uniform current turns out to be somewhat less than if the Fermi sea were swept along with the velocity of the CDW. The effective energy gap for photon absorption is a bit greater than that expected for a band structure based on average energy.

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