

## Back-flow electric current: dc current as a quadratic response to an ac field

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We study the interaction of a running longitudinal wave with a metal. It is shown within a quadratic response that a single wave creates a dc electric current even if the creation of electron-hole pairs is prohibited. As a consequence, a macroscopic electric current depends on an instant distribution of bosons, e.g., plasmons. Beside a formal theory, two practical formulas are provided: the random phase approximation formula for a general electron band structure and a general formula for a single parabolic band.

### I. INTRODUCTION

In this paper we study the interaction of a metal with a single wave having a small but finite amplitude. The wave we assume has a simple sinusoidal shape and propagates along the  $x$  direction. We describe it by a potential  $\phi(x, t) = \phi_q 2 \sin(qx - \omega_q t)$ , where  $\phi_q$  is an amplitude,  $q$  is a wave vector, and  $\omega_q$  is a frequency. Note that this wave does not change its shape, but runs with a phase velocity  $c = \omega_q/q$ . We will call it a running wave to distinguish it from a standing wave  $\sim \sin(qx) \sin(\omega_q t)$ . This distinction is essential in our paper.

The “metal and wave” system is not symmetric with respect to an inversion of coordinates  $x \leftrightarrow -x$ ; therefore one expects that there is a dc electric current in the  $x$  direction. If the wave creates electron-hole pairs, a current undoubtedly exists; this current is usually named according to the origin of the wave, e.g., the acoustoelectric current,<sup>3</sup> the phonon drag,<sup>4</sup> or the photon drag.<sup>5,6</sup> All these effects are described by Boltzmann-like balance equations with currents evaluated from a disturbed distribution of electrons.

According to the balance equation treatment, no current appears if the electron-hole pair creation is excluded. Note that in this case a dielectric function  $\epsilon(\omega_q, q)$  is real and the wave is not absorbed by the metal unless it is in resonance with some collective mode. The following question arises: Does the absence of absorption exclude an induced dc current? We prove in this paper that the answer is *no*. A nonzero dc electric current is also induced by the wave in the absence of absorption. Of course, a theory of this effect has to go beyond the balance equation.

In the theory of plasma, the current in question has been noticed by Fainberg and Shapiro.<sup>1</sup> The theory of this current has been developed by Klíma<sup>2</sup> within classical mechanics and the quasilinear approach. Although most of the properties of metals are given by their cool electron plasma, a similar current has not been reported in the theory of metals. To handle this current in met-

als one should take into account the quantum mechanics and the Pauli principle and, if possible, a nonparabolic band structure, electron-electron correlations beyond the mean field, and a quantization of the driving waves.

Within the theory of plasma, the effect in question is called “the trapping of particles in a monochromatic wave.”<sup>2</sup> This name is tightly connected with the classical mechanics and a dialect used to describe the Landau damping. We prefer to use a dialect related to the theory of metals. Within the dialect of Fermi liquid theory, currents beyond the Boltzmann-like equation are called back flows. Accordingly, we will call this current a wave back flow.

While the wave back flow is not included in the balance equation obtained as a quasiclassical limit of a quantum mechanical description, it can be derived within a classical picture, e.g., from the Vlasov equation. From the classical picture one can see why the wave back flow is missing in the balance equation. Within the Vlasov equation, relative velocities of electrons and the wave are increased in valleys and reduced on tops of the potential; see Ref. 7, Chap. 7.5. Since each electron spends more time in the region of its lower velocity, the averaged relative velocity of the electrons and the wave is reduced. In other words, the electrons drift with the wave and the sum of these drifts constitutes the current in question.

We note that a velocity  $v$  of an electron contributing to the wave back flow is not close to the velocity  $c$  of the wave. An electron with a velocity close to  $c$  contributes to a wave absorption via Landau damping,<sup>7</sup> which corresponds to the drag effect. Indeed, a condition of close velocities  $c \approx v$  is a classical limit of energy conservation for an electron-hole pair creation  $\omega_q \approx vq \approx \hbar^{-1}(\epsilon_{mv+\hbar q} - \epsilon_{mv})$  (where  $\epsilon_k = k^2/2m$ ).

The drag and back flow coexist, if the former is possible. One can see that the wave back flow is not included in the balance equation because the entire interaction of electrons with the wave has been reduced to electron-hole pair creation rates leaving the motion of electrons with  $v \neq c$  aside. Here we want to focus on the wave back

flow; thus we restrict our attention to a case when the electron-hole pair creation is excluded, i.e.,  $v \neq c$  for all electrons.

Until now we have discussed the metal and wave system, where the wave was longitudinal, driven by an external source, and strong enough to be described as classical. Another possibility is to study a “metal and weak wave” system, where one has to take into account that a square of the wave amplitude is quantized. In other words, one can study a dc electric current in a metal with excited bosons. These bosons are plasmons or longitudinal phonons which couple to plasmons via density fluctuations of the electrons. Similarly to the previous case, we are not interested in well-known drag effects,<sup>4</sup> but in wave back flows; therefore we assume only stable bosons which do not decay into electron-hole pairs. Our aim will be to find an electric current as a functional of a boson occupation.

We have organized this paper as follows. In Sec. II we extend the above discussion of the wave back flow within the classical picture and derive the classical value of the wave back flow. This section provides a simplified, classical, quasilinear treatment and it can be read without reference to the many-body Green’s functions. A quantum statistical treatment in the case of the classical wave is included in Sec. III. A more complicated general case of collective modes is discussed in Appendix A. Besides a formal treatment on a level of identities, this section also provides two practical formulas obtained within the random phase approximation. An identity that is useful for a parabolic electron band is in Appendix B. The wave back flow of bosons is discussed in Sec. IV from a weak quantization principle. An exact derivation of the back flow of boson within the quadratic response is in Appendix C.

## II. CLASSICAL WAVE BACK FLOW

As mentioned in the Introduction, the wave back flow can be described using classical mechanics. While the quantum statistic theory is our aim, we start from a classical picture which provides better intuitive insight. Accordingly, in this section we do not put emphasis on the possible generality of our treatment but on its simplicity. From this point of view, this section extends the Introduction.

In the spirit of a Vlasov equation we assume that electrons do not interact mutually, but only with an internal electric field.<sup>7</sup> The wave  $\phi(x, t)$  is a scalar representation of this internal field. To evaluate an induced current we have to derive trajectories of individual electrons and sum their contributions.

### A. Trajectory of a single electron in the presence of a wave

An electron trajectory is given by the Newton equation

$$m \frac{d^2 x}{dt^2} = -\frac{\partial \phi}{\partial x}. \quad (1)$$

A time dependence of the potential can be reduced by a

choice of a running coordinate system given by a substitution  $x = R + ct$ .

We also need an initial condition. To this end we assume that the potential is slowly switched on with a slow exponential increase given by an envelope function  $e^{\eta t}$ ,  $\eta \rightarrow 0$ ; thus  $\phi(x, t) = \phi_q e^{\eta t} 2 \sin(qx - \omega_q t)$ . As an initial condition we use an electron trajectory in the absence of the wave,

$$x_0 = r + vt \quad \text{or} \quad R_0 = r + (v - c)t. \quad (2)$$

We want to solve the Newton equation up to second order in the field amplitude  $\phi_q$ . Thus we write the electron coordinate as  $R = R_0 + R_1 + R_2$ , where the subscript denotes the order, and expand (1):

$$m \frac{d^2 R_1}{dt^2} = -\frac{\partial \phi}{\partial R} \Big|_{R_0} \equiv -\phi_q 2q e^{\eta t} \cos[qr + q(v - c)t], \quad (3)$$

$$m \frac{d^2 R_2}{dt^2} = -R_1 \frac{\partial^2 \phi}{\partial R^2} \Big|_{R_0} \equiv R_1 \phi_q 2q^2 e^{\eta t} \sin[qr + q(v - c)t]. \quad (4)$$

From (3) the linear term results

$$R_1 = \frac{2\phi_q}{mq(v-c)^2} e^{\eta t} \left( \cos[qr + q(v - c)t] - \frac{2\eta}{q(v-c)} \sin[qr + q(v - c)t] \right), \quad (5)$$

where we have neglected higher orders in  $\eta$ . Within the linear approximation the second term in the large parentheses vanishes in the limit  $\eta \rightarrow 0$ , but it brings a nontrivial contribution to the quadratic approximation. Indeed, this second term is proportional to  $\sin[qr + (v - c)t]$  as the second derivative of the potential on the right-hand side of (4). Therefore, on the right-hand side of (4) a nonoscillating term appears:

$$m \frac{d^2 R_2}{dt^2} = -\frac{4\phi_q^2}{m(v - c)^3} \eta e^{2\eta t} + \dots, \quad (6)$$

where the ellipsis stands for oscillating terms. From (6) one can see that besides oscillations, the electron is steadily decelerated; therefore its average velocity  $v_{dc}$  is different from the initial velocity  $v - c$ . At  $t \sim 0$ , the average velocity obtained from (6) reads

$$v_{dc} = v - c - \frac{2\phi_q^2}{m^2(v - c)^3}. \quad (7)$$

According to (7) the velocity of the electron with respect to the wave is reduced within the quadratic approximation. Thus all electrons drift with the running wave, although none of them is trapped. Below [Eq. (15)] we derive a net current by summing over individual electrons. First, we want to discuss the obtained single-electron trajectory in more details.

## B. Integrals of motion

The above straightforward solution of the Newton equation does not provide desirable intuitive insight into a microscopic mechanism of the electron drift. In particular, one might be skeptical about contributions resulting as a reappearance of infinitesimal terms or have an incorrect impression that the shape of the envelope function ( $e^{\eta t}$  above) is crucial for the resulting drift. We find it profitable to recover the electron drift from the integrals of motion. From now on we will not treat electron trajectories, but evaluate the electron velocity  $V(R, t) \equiv dR/dt$  as a function of time and its actual position.

To check that the electron drift does not depend on the envelope function, we take a general function  $K(t)$  instead of  $e^{\eta t}$ ; thus  $\phi(x, t) = \phi_q K(t) 2 \sin(qx - \omega_q t)$ . This function has the following properties:  $K = 1$  for  $t > 0$ ,  $K \rightarrow 0$  for  $t \rightarrow -\infty$ , and  $K$  is smooth, i.e.,  $dK/dt \ll q|v - c|K$ .

From (1), the leading linear term of the electron velocity reads

$$V_1(R, t) = \frac{2\phi_q}{m(v - c)} K(t) \sin(qR). \quad (8)$$

$$\begin{aligned} \left. \frac{\partial \phi(R, t)}{\partial t} \right|_{R_0(t) + R_1(t)} &= \frac{dK}{dt} \phi_q 2 \sin[qR_0(t) + qR_1(t)] \\ &= \frac{dK}{dt} \phi_q 2 \sin[qr + q(v - c)t] + \frac{dK^2(t)}{dt} \frac{\phi_q^2}{m(v - c)^2} 2 \cos^2[qr + q(v - c)t]. \end{aligned} \quad (10)$$

In the integral over time the first term gives a negligible contribution of the order of  $dK/dt(q|v - c|)^{-1}$ . This term corresponds to compensated energy gains and losses along the unperturbed trajectory. The second term reflects the slower velocity of the electron at the potential tops. It has a nonoscillating part due to the cosine square and one finds that the net energy gain is

$$\Delta E = \int_{-\infty}^t dt \frac{\partial \phi}{\partial t} = K^2(t) \frac{\phi_q^2}{m(v - c)^2}. \quad (11)$$

Note that for  $t > 0$  the energy gain does not depend on time ( $K = 1$ ) and its value does not depend on the shape of the envelope function.

Once the potential is switched on, a dynamics of the electron is easy to imagine. The energy of the electron remains constant and the potential is static in the running coordinate system. Now we can conveniently use the energy conservation (9) to find the velocity of the electron as a function of its actual coordinate:

$$V(R) = -\sqrt{(v - c)^2 + \frac{2}{m} [\Delta E - \phi(R)]}. \quad (12)$$

Up to second order in  $\phi$  the velocity reads

One can see that the electron is slower on the tops of the potential and faster in the valleys, therefore the electron spends more time on the tops than in the valleys. As the potential increases, the electron gains a potential energy on the tops and loses it in the valleys; a gain, however, exceeds a loss due to different velocities. A net electron energy is obtained from an integral of motion [multiplying both sides of (1) by  $dR/dt$  and integrating over the time along the electron trajectory]

$$\begin{aligned} \frac{m}{2} V^2(R, t) + \phi(R, t) &= \frac{m}{2} (v - c)^2 \\ &+ \int_{-\infty}^t dt \left. \frac{\partial \phi(R, t)}{\partial t} \right|_{R(t)}. \end{aligned} \quad (9)$$

The left-hand side is a usual sum of actual kinetic and potential energies; the right-hand side includes an initial kinetic energy and a net energy gain  $\Delta E$  (the last term). The net energy gain is explicitly proportional to  $\phi$ ; thus up to the quadratic order it is sufficient to integrate along the electron trajectory within the linear approximation  $R_0(t) + R_1(t) = r + (v - c)t + 2\phi_q q^{-1} m^{-1} (v - c)^{-2} K(t) \cos[qr + q(v - c)t]$ ,

$$\begin{aligned} V(R) &= v - c - \frac{\phi_q 2 \sin(qR)}{m(v - c)} \\ &- \frac{\phi_q^2 2 \sin^2(qR)}{m^2 (v - c)^3} + \frac{\phi_q^2}{m^2 (v - c)^3}. \end{aligned} \quad (13)$$

The last term results from  $\Delta E$ ; the penultimate term results from  $\phi^2$  in an expansion of the square root in (12). In spite of their different origins, the nonoscillating components of the two terms exactly cancel. Accordingly, the perturbation of the velocity as a function of the actual position  $R$  has only oscillating components.

The dc component of the electric current depends only on an average velocity  $v_{dc}$ . To evaluate this average velocity one has to integrate along the electron trajectory. Alternatively, one can obtain the average velocity from the time the electron needs to run over a single period of the potential

$$\frac{1}{v_{dc}} = \frac{q}{2\pi} \int_0^{\frac{2\pi}{q}} \frac{dR}{V(R)} = \frac{1}{v - c} + \frac{2\phi_q^2}{m^2 (v - c)^5}. \quad (14)$$

Within the quadratic approximation, the velocity  $v_{dc}$  obtained from (14) is identical to (7).

Note that the quadratic term of (13) does not contribute to the average velocity in (14). The only contri-

bution results from a square of the linear term; therefore one would obtain the electron drift (7) using simply the linear approximation of the velocity in (14). On the other hand, to keep all quadratic terms under control, the above treatment is necessary. For instance, if one neglects the energy gain  $\Delta E$ , the nonoscillating components of  $V(R)$  do not cancel and one ends up with the wrong factor 3 instead of 2 in (14).

### C. Wave back flow: Net induced current

So far we have discussed a single-electron response. Now we sum over an initial distribution  $f(v)$  of electrons to obtain a net dc current

$$j = -e \int dv f(v)(c + v_{dc}). \quad (15)$$

For simplicity, we assume that the wave velocity  $c$  is much larger than a characteristic electron velocity (whether it be a thermal or Fermi velocity). Then the integral simplifies as

$$j = -\frac{2e}{m^2} \phi_q^2 \int \frac{dv f(v)}{(c-v)^3} \approx -\frac{2eN}{m^2 c^3} \phi_q^2 = -\frac{2eNq^3}{m^2 \omega_q^3} \phi_q^2, \quad (16)$$

where  $N = \int dv f(v)$  is a density of electrons.

Formula (16) can be given a more general form. A polarization operator of an electron gas in the high frequency limit reads [see Ref. 7, Chap. 7.4, or Ref. 8, Eq. (22.14)]

$$\Pi(q, \omega) = \frac{q^2}{m} \int \frac{dv f(v)}{(\omega - qv)^2} \approx \frac{q^2 N}{m \omega^2}; \quad (17)$$

thus formula (16) can be rearranged as

$$j = \frac{eq}{m} \left. \frac{\partial \Pi(q, \omega)}{\partial \omega} \right|_{\omega_q} \phi_q^2. \quad (18)$$

This formula was first derived by Klíma; see the second term of formula (3.6) in Ref. 2. It is very easy to apply and in fact it is very general. We will recover (18) within the quantum statistics and specify its range of validity in Sec. III.

### D. Relation of the wave back flow to wave momentum

The general validity of formula (18) follows from the relation between the density of momentum of the wave and the electric current. The current relates to a velocity as  $j \sim -ev$  and the momentum relates as  $Q \sim mv$ ; thus the current is proportional to an electronic share of a momentum density

$$j = -\frac{e}{m} Q_{el}. \quad (19)$$

It is easy to check that this interpretation of the wave back flow holds for plasmons in three-dimensional (3D) metals. A longitudinal electric field of plasmons does not carry any momentum, therefore the electronic share  $Q_{el}$  represents a total density of momentum in this particular case. The total momentum density can be evaluated directly from the energy density  $W = q^2 \phi_q^2 / (2\pi e^2)$  (see Ref. 7) because  $Q_{el} = qW/\omega_q$ . Using a dispersion relation of 3D plasmons,  $\omega_q = \omega_P = \sqrt{4\pi N e^2 / m}$ , from (19) one recovers (16).

Let us briefly summarize this section. Although not trapped, electrons of the metal drift with the running wave because their velocities with respect to the wave are reduced within the quadratic approximation. Velocity changes of individual electrons are rather small, but, on the other hand, all electrons take part in this motion. This electric current can also be interpreted in terms of the momentum share carried by the electrons. This is a physical reason why the current can be easily expressed in terms of the polarization operator and why formula (18) will turn out to be general. We note that the relation between the momentum density and the current follows from a parabolic band structure, which is inevitable for Newtonian physics, but not for quantum mechanics.

## III. WAVE BACK FLOW: QUANTUM STATISTICS

In this section we derive the wave back flow (i.e., the dc electric current driven by an ac field) within the quantum statistics. As we have shown in the preceding section, the wave back flow is a quadratic effect; therefore we start our treatment from formal quadratic response theory. For simplicity we assume that the system was in the ground state  $|G\rangle$  at  $t \rightarrow -\infty$ .

In Sec. II, we studied a motion of electrons driven by the internal field  $\phi$ . Formal response theory, however, has to start from some external field  $\varphi$ . The internal field  $\phi$  will result as a part of the system response.

### A. Quadratic response

The time evolution of a system is described by a  $U$  matrix defined by an expansion in an interaction representation [see Ref. 9, above Eq. (8-6)]

$$U(t_0) = 1 - i \int_{-\infty}^{t_0} dt \hat{\varphi}_I(t) - \int_{-\infty}^{t_0} dt \hat{\varphi}_I(t) \int_{-\infty}^t dt' \hat{\varphi}_I(t'), \quad (20)$$

where we have left orders beyond quadratic. An electric current is given by a mean value of a homogeneous current density operator  $\hat{j}_I(t_0)$ ,

$$j(t_0) = \langle G | U^{-1}(t_0) \hat{j}_I(t_0) U(t_0) | G \rangle, \quad (21)$$

and its quadratic component is

$$\begin{aligned}
j(t_0) = & \int_{-\infty}^{t_0} dt \int_{-\infty}^{t_0} dt' \langle G | \hat{\varphi}_I(t') \hat{j}_I(t_0) \hat{\varphi}_I(t) | G \rangle \\
& - \int_{-\infty}^{t_0} dt \int_{-\infty}^t dt' \langle G | \hat{\varphi}_I(t') \hat{\varphi}_I(t) \hat{j}_I(t_0) | G \rangle \\
& - \int_{-\infty}^{t_0} dt \int_{-\infty}^t dt' \langle G | \hat{j}_I(t_0) \hat{\varphi}_I(t) \hat{\varphi}_I(t') | G \rangle. \quad (22)
\end{aligned}$$

The three-time functions in the integrands have to be evaluated perturbatively. This is quite a demanding task because an electron-electron interaction (so far hidden in an unperturbed Hamiltonian) makes a time dependence of the field operators  $\hat{\varphi}_I$  nontrivial. To handle this task we employ the Green's function machinery.

### B. Imposed undamped wave

In this subsection we show that under the condition that the wave vector  $q$  and frequency  $\omega_q$  are such that the external field  $\varphi$  does not create any excitation in the metal, it is possible to evaluate formula (22) with the help of zero-temperature causal Green's functions. Of course, this condition is too restrictive for practical applications because large amplitudes of waves can be achieved only if  $\omega_q$  and  $q$  belong to some collective excitation of the metal. Moreover, a wave back flow of bosons is excluded by this condition. In practice, this restriction is not so bad. In the classical picture we have found that electric current is given by the derivative of the polarization operator, which is a smooth function of  $q$  and  $\omega$  in the vicinity of collective modes. It is the singular relation of the internal field  $\phi$  and the external field  $\varphi$  that requires us to distinguish the collective modes. If we approach the collective mode keeping a constant amplitude of  $\phi$  (not of  $\varphi$ ), the collective mode does not represent any special point. Therefore, the formula we derive here applies also to collective modes. More details are in Appendix A, which should be read after this section.

Our derivation of the system response is based on the fluctuation-dissipation theorem. While the use of the fluctuation-dissipation theorem is complicated for a general quadratic response because of a rich analytic structure, in the case of the homogeneous current there is a simplification which follows from the fact that the ground state is an eigenstate of the homogeneous current density operator with zero as an eigenvalue

$$\hat{j}_I(t_0)|G\rangle = 0. \quad (23)$$

Accordingly, only the first term of (22) contributes and there is only a single important analytic piece. This simplification corresponds to what we have seen already in the classical picture, that the wave back flow can be obtained from the linear perturbation of the electron trajectory.

As mentioned, we want to use a zero-temperature causal Green's function to evaluate the first term of (22). Apparently, the order of the operators does not correspond to a time ordering on a real time axis because  $\hat{\varphi}_I(t')$  stands on the left-hand side of  $\hat{j}_I(t_0)$  and  $t' < t_0$ .

We introduce the causal Green's function into (22) by extending the  $t'$  integration to infinity and subtracting the proper part

$$\begin{aligned}
j(t_0) = & \int_{-\infty}^{t_0} dt \int_{-\infty}^{\infty} dt' \langle G | \hat{\varphi}_I(t') \hat{j}_I(t_0) \hat{\varphi}_I(t) | G \rangle \\
& - \int_{-\infty}^{t_0} dt \int_{t_0}^{\infty} dt' \langle G | \hat{\varphi}_I(t') \hat{j}_I(t_0) \hat{\varphi}_I(t) | G \rangle. \quad (24)
\end{aligned}$$

The second term has the causal ordering on the real time axis; we will show that the first term vanishes if the field does not create any excitation of the metal.

To prove that the first term of (24) vanishes, we insert a unity operator  $1 = |G\rangle\langle G| + \sum_E |E\rangle\langle E|$  between  $\hat{\varphi}_I(t')$  and  $\hat{j}_I(t_0)$ . Here  $|E\rangle$  is an excited eigenstate with the excitation energy  $E$ . According to (23), the ground state does not contribute; thus we can focus on excited states. The time integral over the whole time axis results into a  $\delta$  function

$$\int_{-\infty}^{\infty} dt' \langle G | \hat{\varphi}_I(t') | E \rangle \sim 2\pi\delta(\omega_q - E), \quad (25)$$

which is nonzero only if the transition to the state  $|E\rangle$  is possible. According to the assumption that the field does not create any excitation, no such state exists; therefore the left-hand side of (25) is zero and the first term in (24) vanishes.

Formula (24) with the first term eliminated provides the current in terms of an element of a causal Green's function. A convenient use of causal Green's functions, however, requires all limits of time integrals to be fully determined by the time ordering. To this end we use a symmetry with respect to  $t$  and  $t'$ ,

$$\begin{aligned}
j(t_0) = & -\frac{1}{2} \int_{-\infty}^{t_0} dt \int_{t_0}^{\infty} dt' \langle G | \hat{\varphi}_I(t') \hat{j}_I(t_0) \hat{\varphi}_I(t) | G \rangle \\
& - \frac{1}{2} \int_{t_0}^{\infty} dt \int_{-\infty}^{t_0} dt' \langle G | \hat{\varphi}_I(t) \hat{j}_I(t_0) \hat{\varphi}_I(t') | G \rangle, \quad (26)
\end{aligned}$$

and Eq. (23) to add integrals where both field operators stand at the same side of the current operator. Finally one finds that the current reads

$$j(t_0) = -\frac{1}{2} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' \langle G | T_c \hat{\varphi}_I(t') \hat{j}_I(t_0) \hat{\varphi}_I(t) | G \rangle, \quad (27)$$

where  $T_c$  is Dyson time-ordering operator on a real time axis. From now on, all time integrals run from  $-\infty$  to  $\infty$ .

To make the structure of the response formula more explicit, we express the external field operator  $\varphi_I$  in terms of a local density operator  $\hat{n}_I$

$$\hat{\varphi}_I(t) = \int dx \hat{n}_I(x, t) \varphi(x, t), \quad (28)$$

so that formula for the current reads

$$\begin{aligned}
j(t_0) = & -\frac{1}{2} \int dx dt dx' dt' \varphi(x', t') \varphi(x, t) \\
& \times \langle G | T_c \hat{n}_I(x', t') \hat{j}_I(t_0) \hat{n}_I(x, t) | G \rangle. \quad (29)
\end{aligned}$$

From now on we can make use of the machinery of the Green's functions. We introduce an  $S$  matrix defined by ( $\hat{H}$  is the full Hamiltonian of the system except for the external field)

$$S = T_c \exp -i \int dt \hat{H}(t), \quad (30)$$

and express (29) in Heisenberg representation with help of the Green's function as<sup>8</sup>

$$j(t_0) = -\frac{1}{2} \int dx dt dx' dt' \varphi(x', t') \varphi(x, t) \times \frac{\langle 0 | T_c \hat{n}(x', t') \hat{j}(t_0) \hat{n}(x, t) S | 0 \rangle}{\langle 0 | S | 0 \rangle}. \quad (31)$$

Here  $|0\rangle$  is the ground state of the noninteracting system. This formula can already be treated by Green's-function techniques.

### C. Translation invariance and stationarity

Formula (31) is still not suited for practical applications because of the three-time operator, which is usually difficult to evaluate. Here we use stationarity and translational invariance to express the three-time operator in terms of a two-time operator, a density-density response.

Due to translational invariance, the function  $\langle G | T_c \hat{n}(x', t') \hat{j}(t_0) \hat{n}(x, t) | G \rangle$  is a function of the coordinate difference  $r = x - x'$ . The integration over the "center of mass" coordinate  $R = (x + x')/2$  can be performed separately on the potential square

$$\varphi^{(2)}(r; t', t) = \frac{1}{\Omega} \int dR \varphi(R + r/2, t) \varphi(R - r/2, t'), \quad (32)$$

where  $\Omega$  is a sample volume.

For the potential of the single running wave  $\varphi(x, t) = \varphi_q 2 \sin(qx - \omega_q t)$ , a homogeneous component of the field squared is

$$\varphi^{(2)}(r, \tau) = \varphi_q^2 2 \cos(qr - \omega_q \tau), \quad (33)$$

where  $\tau = t - t'$ . From (33) one can see that  $\varphi^{(2)}$  also does not depend on the center of mass time  $T = (t + t')/2$ , i.e.,  $\varphi^{(2)}$  is stationary. Equation (31) thus simplifies to

$$j(t_0) = -\frac{\Omega}{2} \int dr d\tau dT \varphi^{(2)}(r, \tau) \times \frac{\langle 0 | T_c \hat{n}(0, T - \tau/2) \hat{j}(t_0) \hat{n}(r, T + \tau/2) S | 0 \rangle}{\langle 0 | S | 0 \rangle}. \quad (34)$$

The function  $\langle 0 | T_c \hat{n}(0, T - \tau/2) \hat{j}(t_0) \hat{n}(r, T + \tau/2) S | 0 \rangle$  does not depend on the choice of the initial time; therefore the center of mass can be moved into the time argument of the current operator

$$\int dT \langle 0 | T_c \hat{n}(0, T - \tau/2) \hat{j}(t_0) \hat{n}(r, T + \tau/2) S | 0 \rangle = \int dT \langle 0 | T_c \hat{n}(0, 0) \hat{j}(T) \hat{n}(r, \tau) S | 0 \rangle. \quad (35)$$

The integral over all time arguments of the current operator allows for a remarkable simplification. If we include an infinitesimal, homogeneous, stationary vector potential  $A$  into the Hamiltonian of the  $S$  matrix, not into the ground state  $|0\rangle$ , the current operator can be expressed as  $[H \sim \epsilon_k - eA]$ ; see Ref. 8, Eq. (19.2), and above]

$$\hat{j}(T) = \frac{1}{\Omega} \frac{\partial \hat{H}(T)}{\partial A}. \quad (36)$$

Accordingly, the time integral of the current operator can be generated from the  $S$  matrix,

$$T_c \int dT \hat{j}(T) S = \frac{i}{\Omega} \frac{\partial S}{\partial A}. \quad (37)$$

This allows us to express the current with the help of the partial derivative of a two-time function

$$j = \frac{1}{2} \int dr d\tau \varphi^{(2)}(r, \tau) \frac{\partial}{\partial A} \frac{\langle 0 | T_c \hat{n}(0, 0) \hat{n}(r, \tau) S | 0 \rangle}{i \langle 0 | S | 0 \rangle}. \quad (38)$$

The Green's function in the integral is a common density-density response function<sup>10</sup>

$$K(r, t) = \frac{\langle 0 | T_c \hat{n}(0, 0) \hat{n}(r, \tau) S | 0 \rangle}{i \langle 0 | S | 0 \rangle}. \quad (39)$$

In contrast to the quadratic response, the theory of the density-density response is already well established and we will make use of it. Before we do so we use the explicit form of  $\varphi^{(2)}$  to turn formula (38) into the energy-momentum representation

$$j = \frac{1}{2} \varphi_q^2 \frac{\partial}{\partial A} [K(q, \omega_q) + K(-q, -\omega_q)]. \quad (40)$$

The density-density response function obeys a boson symmetry  $K(-q, -\omega) = K(q, \omega)$ , which follows from its definition, independent of the presence of a symmetry-breaking vector potential  $A$ . Therefore we have obtained

$$j = \varphi_q^2 \frac{\partial K(q, \omega_q)}{\partial A}. \quad (41)$$

This formula is already suitable for applications. With respect to collective modes, however, it is better to rearrange (41) in terms of the polarization operator.

### D. Quadratic response in terms of the polarization

A perturbative expansion of the density-density response can be reduced to a perturbative expansion of a polarization operator<sup>10</sup>

$$K(q, \omega) = \Pi(q, \omega) + \Pi(q, \omega) D_0(q, \omega) K(q, \omega), \quad (42)$$

where  $D_0$  is a bare boson Green's function, whether it is a Coulomb interaction or a phonon Green's function with interaction vertices included (we assume only the local interaction), or both combined.

From (42) the derivative of  $K$  gives

$$\frac{\partial K(q, \omega)}{\partial A} = \frac{\partial \Pi(q, \omega)}{\partial A} \varepsilon^{-2}(q, \omega), \quad (43)$$

where  $\varepsilon$  is a dielectric function

$$\varepsilon(q, \omega) = 1 - D_0(q, \omega)\Pi(q, \omega). \quad (44)$$

Now we substitute (43) into (41) and obtain the final formula

$$j = \phi_q^2 \frac{\partial \Pi(q, \omega_q)}{\partial A}, \quad (45)$$

where we have substituted the external field by the internal one via the relation  $\phi_q = \varphi_q/\varepsilon(q, \omega_q)$ .

Formula (45) is our final result. With respect to its application, the only required input is the derivative of the polarization operator. The polarization operator  $\Pi(q, \omega_q)$  is real because of excluded electron-hole pair creation, thus one can use any formula for the polarization operator at hand [ $\text{Re} \Pi_c(\omega, q) = \text{Re} \Pi_R(\omega, q) = \text{Re} \Pi_A(\omega, q)$ ; see Ref. 8, Eq. (7.25)]. This formula is the desired quantum statistical generalization of the classical formula (18).

### E. Wave back flow in the random phase approximation

So far we have not made any approximation except for the zero temperature limit and quadratic order of the response. Here we demonstrate the use of (45) for the simplest case, the random phase approximation (RPA).

With a gauge  $A$  the kinetic energy of the electron is  $\varepsilon_{k-eA}$ . The vector potential  $A$  does affect the ground state  $|0\rangle$ . Accordingly, the occupation numbers of individual single-electron states are independent of  $A$  and the RPA polarization operator reads

$$\Pi(q, \omega_q) = \int \frac{dk}{(2\pi)^d} \frac{f_k - f_{k+q}}{\omega_q + \varepsilon_k - \varepsilon_{k+q}}. \quad (46)$$

Taking the derivative at  $A = 0$  one finds

$$\begin{aligned} \frac{\partial \Pi(q, \omega_q)}{\partial A} &= e \int \frac{dk}{(2\pi)^d} \left( \frac{\partial \varepsilon_k}{\partial k} - \frac{\partial \varepsilon_{k+q}}{\partial k} \right) \\ &\quad \times \frac{f_k - f_{k+q}}{(\omega_q + \varepsilon_k - \varepsilon_{k+q})^2}. \end{aligned} \quad (47)$$

Except for special cases this formula has to be treated numerically. For the numerical integration it might be advantageous to rearrange (47) into an equivalent form, using integration by parts. Then the back-flow current results:

$$j = -e\phi_q^2 \int \frac{dk}{(2\pi)^d} \frac{1}{\omega_q + \varepsilon_k - \varepsilon_{k+q}} \frac{\partial}{\partial k} (f_k - f_{k+q}). \quad (48)$$

Formula (48) shows that the only contributing electronic states are in a  $q$  vicinity of the Fermi surface.

### F. Wave back flow for the parabolic electron band

For metals with a parabolic electron band, one can make use of momentum conservation to simplify the back-flow current (45) to formula (18). Here we confirm formula (18) within the RPA. For the parabolic band

$\varepsilon_k = k^2/2m$ , the velocity difference in (47) is independent of the electron momentum

$$\frac{\partial \varepsilon_k}{\partial k} - \frac{\partial \varepsilon_{k+q}}{\partial k} = -\frac{q}{m}. \quad (49)$$

The square in the denominator of (47) can be expressed as the derivative with respect to the frequency

$$\frac{1}{(\omega + \varepsilon_k - \varepsilon_{k+q})^2} = -\frac{\partial}{\partial \omega} \frac{1}{\omega + \varepsilon_k - \varepsilon_{k+q}}; \quad (50)$$

therefore one finds that

$$\frac{\partial \Pi(q, \omega_q)}{\partial A} = \frac{eq}{m} \left. \frac{\partial \Pi(q, \omega)}{\partial \omega} \right|_{\omega_q}. \quad (51)$$

Substituting (51) into (45) one recovers (18).

Formula (51) is a direct consequence of momentum conservation; therefore it applies for any approximation of the polarization operator. A general proof of (51) is given in Appendix B. The form (18) might be particularly useful for low-dimensional metals prepared on semiconductor surfaces, where the electron concentration is too low to guarantee the validity of the RPA, while a parabolic approximation of the band is usually sufficient.

## IV. WAVE BACK FLOW OF BOSONS

Let us assume a stable boson which cannot decay into an electron-hole pair. The wave back flow has a straightforward consequence: this boson is accompanied by an electric current. Here we evaluate its value.

In principle, the wave back flow of bosons can be treated within the quadratic response theory. An external field tuned to a selected collective mode creates corresponding bosons. After the external field is switched off, these bosons persist, causing the wave back flow in question. Apparently, the process has two stages: the creation of an excess occupation  $\Delta N_q^\alpha$  of boson modes and the observation of the current  $j[\Delta N_q^\alpha]$ , a functional of the occupation. Here we are interested only in the second part of the problem, the functional  $j[\Delta N_q^\alpha]$ . The boson distribution  $\Delta N_q^\alpha$  is an input of our treatment.

### A. Weak quantization approach

A straightforward approach to evaluate the dc electric current is the following: associate a potential wave  $\phi$  to a single boson; apply the quadratic response formula (45) and sum over all bosons.

The internal potential  $\phi$  of a single boson is not well defined. A phase of this wave is arbitrary and its amplitude  $\phi_q^\alpha$  is inversely proportional to the square root of a sample volume  $\Omega$ ; thus  $\phi_q^\alpha \rightarrow 0$  in the thermodynamic limit  $\Omega \rightarrow \infty$ . According to (45), however, the quadratic response depends only on the averaged potential square where the unknown phase is irrelevant and an inconvenience of the thermodynamic limit can be avoided normalizing  $\phi_q^\alpha$  to a unitary volume similarly as a boson

distribution.

To identify  $\phi_q^\alpha$ , we use the weak quantization principle and take the potential  $\phi$  as an operator in the second quantization. The average potential square  $\phi^2$  then becomes a potential-potential correlator, i.e., a part of a screened boson Green's function  $D$ .

### B. Potential-potential correlator

Now we specify  $D[\Delta N]$  as a functional of an excess occupation. For simplicity,  $\Delta D$  is a deviation of the Green's function and  $D$  is an equilibrium (zero temperature) value.

We describe the equilibrium part first. Boson dispersion relations  $\omega_q^\alpha$ , where  $\alpha$  denotes branches, are given by [for modes with an infinite lifetime  $D(q, \omega)$  is real]

$$D^{-1}(q, \omega_q^\alpha) = 0. \quad (52)$$

Each mode is thus represented by a pole of the Green's function; this pole has a weight  $Z_q^\alpha$  given by

$$\frac{1}{Z_q^\alpha} = \left. \frac{\partial D^{-1}(q, \omega)}{\partial \omega} \right|_{\omega_q^\alpha}. \quad (53)$$

We call  $Z_q^\alpha$  a norm of the mode.

Now we find  $\Delta D$ . For free bosons the occupation numbers enter the Green's function as factors of corresponding poles; therefore a dominant contribution to  $\Delta D$  reads

$$\begin{aligned} \Delta D(r, \tau) &\approx -i\phi^{(2)}(r, \tau) \\ &\equiv -i \sum_{\alpha} \int \frac{dq}{(2\pi)^d} Z_q^\alpha \left( \Delta N_q^\alpha e^{iqr - i\omega_q^\alpha \tau} \right. \\ &\quad \left. + \Delta N_{-q}^\alpha e^{iqr + i\omega_q^\alpha \tau} \right), \end{aligned} \quad (54)$$

where  $d$  is a system dimension and the equivalence defines the function  $\phi^{(2)}$ .

The form (54) with mixed  $q$  and  $-q$  terms is suitable for the momentum representation; alternatively one can substitute  $q \rightarrow -q$  in the second term, which yields  $\phi^{(2)}$  as a sum over running waves:

$$\phi^{(2)}(r, \tau) = \sum_{\alpha} \int \frac{dq}{(2\pi)^d} Z_q^\alpha \Delta N_q^\alpha 2 \cos(qr - \omega_q^\alpha \tau). \quad (55)$$

The factor  $Z_q^\alpha \Delta N_q^\alpha$  corresponds to a square of the potential [see (33)]; therefore

$$\phi_q^\alpha = \sqrt{Z_q^\alpha \Delta N_q^\alpha}. \quad (56)$$

### C. Wave back flow

Now we are ready to use formula (45). Substituting from (56) we find that the current is

$$j = \sum_{\alpha} \int \frac{dq}{(2\pi)^d} Z_q^\alpha \Delta N_q^\alpha \frac{\partial \Pi(q, \omega_q^\alpha)}{\partial A}. \quad (57)$$

This formula is the desirable functional  $j[\Delta N]$ .

The above derivation has a few shortcomings. First, because of the presence of nonequilibrium bosons, one can be skeptical about the use of the zero temperature Green's function. Second, the potential-potential correlator has a much richer structure and it is not clear how to deal with its off-pole parts. Third, quadratic responses to quantum and classical screened fields are not exactly identical because of mutual correlations in the quantum case. All these points are fixed using nonequilibrium Green's functions and formula (57) is recovered as an exact result. Because of its rather technical nature, this proof is given in Appendix C.

### D. Wave back flow and the density of momentum in jellium

From (57) one can see that plasmons carry a dc electric current. This conclusion met a lot of complains based on a common prejudice that the only motion of electrons induced by plasmons is an oscillation with the plasma frequency. This prejudice contradicts the momentum conservation law, which requires the existence of a term like (57). We demonstrate this relation of the wave back flow and the momentum conservation on the simplest system, the jellium model without phonons.

For the jellium model, formula (57) can be remarkably simplified. Since the electron band is parabolic, the derivative of the polarization operator with respect to the vector potential simplifies to the energy derivative; see (51). In the absence of phonons, there is a single boson branch, the plasmons, thus we suppress the superscript  $\alpha$ . The norm  $Z_q$  follows from the inverse dressed Green's function  $D^{-1}(q, \omega) = V_q^{-1} - \Pi(q, \omega)$ , where  $V_q$  is a Coulomb potential. The Coulomb interaction is instant ( $V_q$  is independent of  $\omega$ ); therefore the denominator in (53) depends only on the polarization operator and  $Z_q^{-1} = -\partial \Pi / \partial \omega$ . The product  $Z_q \partial \Pi / \partial A$  thus does not depend on the polarization operator and from (57) one finds that the wave back flow is proportional to the density of momentum  $Q$ ,

$$j = -\frac{e}{m} \int \frac{dq}{(2\pi)^d} q \Delta N_q = -\frac{e}{m} Q. \quad (58)$$

This simple relation is not accidental but follows directly from definitions of the current and momentum density operators:

$$\hat{j} = -\frac{e}{m} \int \frac{dk}{(2\pi)^d} k \psi_k^\dagger \psi_k, \quad \hat{Q} = \int \frac{dk}{(2\pi)^d} k \psi_k^\dagger \psi_k. \quad (59)$$

Here  $\psi_k^\dagger$  is the creation operator of the bare electron with momentum  $k$ . According to (59) the homogeneous electric current  $j$  and the homogeneous density of momentum  $Q$  are identical, except for the factor  $-e/m$ .

In terms of single-particle excitations, the total momentum density depends on both a quasielectron distribution  $f_k$  and the plasmon distribution  $N_q$ ,

$$Q = \int \frac{dk}{(2\pi)^d} k f_k + \int \frac{dq}{(2\pi)^d} q N_q. \quad (60)$$



Thus the current is

$$j = -\frac{e}{m} \int \frac{dk}{(2\pi)^d} k f_k - \frac{e}{m} \int \frac{dq}{(2\pi)^d} q N_q. \quad (61)$$

The first term is a common current term used in the Landau theory of Fermi liquids. The bare electron mass  $m$  in the factor  $-e/m$  is known to result from compensations of a group velocity renormalization and a quasiparticle back flow. In our case the quasiparticle distribution remains in equilibrium and this term is zero. The second term is the wave back flow derived above.

It is our feeling that the wave back flow of plasmons is a natural part of Fermi liquid theory because it reflects the momentum conservation law in a way similar to the quasiparticle back flow. In standard metals typical energies of plasmons are  $\sim 1$  eV; therefore plasmons are not excited either thermally or by fields slowly varying in time and space. Accordingly, former theories of metals left nonequilibrium plasmons aside. In more recently studied 2D metals, the plasmons dispersion relation has square root behavior for small momenta;<sup>11</sup> therefore 2D plasmons are never frozen out.

## V. CONCLUSIONS

We have shown that a running wave in metals creates a dc current of a back-flow nature; we call this current a wave back flow. The amplitude of this current is proportional to the square of the field strength and the direction is identical to the wave vector, unless the metal is anisotropic.

An important feature of our theory is that it is formulated in terms of a polarization operator which provides the convenient final formula (45). A particularly simple formula (18) holds for a single parabolic electron band.

For the sake of simplicity we have derived the wave back flow at the zero temperature. The classical case, however, shows that at finite temperatures the wave back flow also appears. We expect that the only modification of the quantum statistical formula (45) will be covered by the temperature dependence of the polarization operator  $\Pi(q, \omega)$ .

An interesting question is under which conditions the wave back flow could be observed. With reservations that we are not fully familiar with recent experimental capabilities, it is our feeling that two-dimensional systems are more promising than the normal three-dimensional metals. This is because the two-dimensional metal can be easily penetrated by a driving field from the orthogonal direction, and the driving field can be modulated by a grid.<sup>12</sup>

It is also advisable to use a field with a wave vector and a frequency from a plasma dispersion relation. Indeed, the inverse dielectric function  $\epsilon_R^{-1}(q, \omega_q)$  diverges at the plasma mode; thus the internal field reaches its maximum value, while the polarization operator in a high frequency range is a smooth function.

We have also shown that plasmons (or longitudinal bosons coupled to them) contribute to the dc electric current even if they do not create electron-hole pairs.

Accordingly, the current density as a functional of distributions of elementary excitations includes a term which is odd (linear in this paper) in the boson distribution and even in the quasielectron distribution. For the jellium model, this term was shown to be consistent with the relation between the total density of momentum and the density of current.

Similarly to the back flow of a classical wave, 2D metals are promising to have a demonstrable wave back flow of plasmons. We note that unlike the classical wave which has to be driven by a laser light, the plasmons can be created by an incoherent light or other sources.

In principle, there are also contributions of the wave back flow of bosons to the thermoelectric and acoustoelectric effects. We are not in a position, however, to provide reliable estimates of their magnitudes.

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## APPENDIX A: WAVE BACK FLOW IN COLLECTIVE MODES

In Sec. III we derived the wave back flow assuming that the wave is not in resonance with any internal collective mode. Here we extend this derivation to collective modes.

The explicit time integration limits of (22) are inconvenient for formal manipulations. To make the time integration limits implicit, we follow Kadanoff and Baym<sup>9</sup> and introduce a closed time path from  $-\infty$  to  $t_0$  and back to  $-\infty$ . The order of operators in all terms on the right-hand side of (22) is identical to the time order on this close path; therefore (22) can be expressed as

$$j(t_0) = -\frac{1}{2} \oint dt \int dt' \langle G|T \hat{j}_I(t_0) \hat{\varphi}_I(t) \hat{\varphi}_I(t')|G\rangle. \quad (A1)$$

Here  $T$  is the time ordering operator on the closed path, the factor  $1/2$  compensates both time integrals running twice along the real time axis, and the signs of individual analytical elements are given by the direction of the time integration.

To be fully consistent with Kadanoff and Baym one can extend the time integration into complex times. These two formulations are identical in the zero temperature limit because the statistical operator  $\rho = e^{-\beta \hat{H}} / \text{Tr}(e^{-\beta \hat{H}})$  goes to  $|G\rangle\langle G|$  as the inverse temperature increases  $\beta \rightarrow \infty$ .

### 1. Functional derivatives

Now we express (A1) in terms of functional derivatives. First, we introduce a generating functional

$$L = i \left\langle G \left| T \exp \left( -i \oint d\tau \hat{H}_A(\tau) + \hat{\varphi}(\tau) \right) \right| G \right\rangle, \quad (\text{A2})$$

where all operators are in the Schrödinger representation. The electron kinetic energy includes a homogeneous but time-dependent vector gauge  $A(t)$ ,  $H_k(t) = \epsilon_{k-eA(t)}$ . One can also use  $L = i \langle TS \rangle$  from Eq. (5-1) in Ref. 9.

A functional derivative with respect to the vector potential generates the homogeneous current density oper-

ator; see Ref. 8 Eq. (19.2), and above. This can be seen from a perturbation of  $H$  by a small vector potential

$$\delta \oint d\tau H_k(\tau) = -e \frac{\partial \epsilon_k}{\partial k} \oint d\tau \delta A(\tau). \quad (\text{A3})$$

A sum of  $-e \partial \epsilon_k / \partial k$  over all momenta  $k$  provides the homogeneous current density multiplied by the volume  $\Omega$  of the sample, thus  $\Omega^{-1} \delta \oint \hat{H} / \delta A(t) = \hat{j}(t)$ . From a derivative of the generating functional one finds

$$\begin{aligned} \frac{1}{\Omega} \frac{\delta L}{\delta A(t)} &= \frac{1}{\Omega} \left\langle G \left| T \exp \left( -i \oint d\tau \hat{H}(\tau) + \hat{\varphi}(\tau) \right) \frac{\delta \oint d\tau' \hat{H}(\tau')}{\delta A(t)} \right| G \right\rangle \\ &= \left\langle G \left| T \exp \left( -i \oint d\tau \hat{H}(\tau) + \hat{\varphi}(\tau) \right) \hat{j}(t) \right| G \right\rangle. \end{aligned} \quad (\text{A4})$$

The external field can be also expressed in terms of the functional derivatives. From the explicit expression for the operator of the external field

$$\oint d\tau \hat{\varphi}(\tau) = \oint d\tau \int dx \hat{n}(x, \tau) \varphi(x, \tau) \equiv \hat{n}(\bar{1}) \varphi(\bar{1}), \quad (\text{A5})$$

where  $\hat{n}$  is a operator of the local density, one finds  $\delta \oint \hat{\varphi} / \delta \varphi(1) = \hat{n}(1)$ . The last part of (A5) introduces a reduced notation: the number is a cumulative variable  $1 \equiv x_1, t_1$  and the integration denoted by the overbar includes the time integral on the closed path.

With the help of functional derivatives given by (A4) and (A5), Eq. (A1) can be rearranged as

$$j(t_0) = \frac{1}{2\Omega} \varphi(\bar{2}) \varphi(\bar{1}) \frac{\delta}{\delta A(t_0)} \frac{\delta^2 L}{\delta \varphi(\bar{2}) \delta \varphi(\bar{1})}. \quad (\text{A6})$$

This form of the quadratic response is a very convenient starting point for a perturbative treatment.

## 2. Quadratic response in terms of polarization

In general, the functional derivatives in (A6) can be performed in any order and the same equation (A1) results. On the other hand, if one combines the functional derivatives with a perturbative expansion, the order of derivatives determines the character of the perturbative treatment. For instance, if one takes first the derivative with respect to the vector potential, the single-electron Green's function results. This single-electron Green's function can be expressed in terms of the transport equation and one arrives at a transport equation treatment. If one starts from the functional derivatives with respect to the fields and uses the perturbative expansion before the derivative with respect to the vector potential, the resulting formulation is quite different. Indeed, the second derivative of the generating functional with respect to the fields is the density-density response function<sup>10</sup>

$$K(1, 2) = \frac{\delta^2 L}{\delta \varphi(2) \delta \varphi(1)}, \quad (\text{A7})$$

which is a function typical of the linear response theory.

Similarly to Sec. III, the perturbative expansion of the density-density response can be reduced to the perturbative expansion of the polarization operator<sup>10</sup>

$$K(1, 2) = \Pi(1, 2) + \Pi(1, \bar{3}) D_0(\bar{3}, \bar{4}) K(\bar{4}, 2). \quad (\text{A8})$$

The functional derivative of  $K$  from (A8) results

$$\frac{\delta K(1, 2)}{\delta A(t_0)} = \frac{\delta \Pi(\bar{3}, \bar{4})}{\delta A(t_0)} \varepsilon^{-1}(\bar{4}, 2) \varepsilon^{-1}(\bar{3}, 1), \quad (\text{A9})$$

where

$$\varepsilon(1, 2) = \delta(1 - 2) - D_0(1, \bar{3}) \Pi(\bar{3}, 2). \quad (\text{A10})$$

Now we substitute (A9) into (A6) and obtain the final formula

$$j(t_0) = \frac{1}{2\Omega} \frac{\delta \Pi(\bar{3}, \bar{4})}{\delta A(t_0)} \varepsilon^{-1}(\bar{3}, \bar{1}) \varphi(\bar{1}) \varepsilon^{-1}(\bar{4}, \bar{2}) \varphi(\bar{2}). \quad (\text{A11})$$

## 3. Internal fields

So far, the response has been expressed in terms of the external field, while we need the internal field to make a limit into the collective mode. The internal field is given by the screening of the external field

$$\phi(1) = \varepsilon^{-1}(1, \bar{2}) \varphi(\bar{2}). \quad (\text{A12})$$

To make contact with a common retarded relation between the external and internal fields, we convert the integral on the close time path to the integral on the real time axis; see Appendix A in Ref. 13,

$$\phi(1) = \int_{-\infty}^{\infty} dt_2 \varepsilon_R^{-1}(1, \bar{2}) \varphi(\bar{2}). \quad (\text{A13})$$

According to (A11) and (A12) the wave back flow can be expressed in terms of the internal fields

$$j(t_0) = \frac{1}{2\Omega} \phi(\bar{2}) \phi(\bar{1}) \frac{\delta \Pi(\bar{1}, \bar{2})}{\delta A(t_0)}. \quad (\text{A14})$$

This formula can be evaluated for the fields which are not tuned to any collective mode using the theory developed in Sec. III. Since the collective mode does not represent any special point for the polarization operator, one can see that formulas developed in Sec. III hold also for collective modes.

## APPENDIX B: PARABOLIC BAND

In this appendix we prove that (51) holds exactly for the parabolic electron band and instant (nonretarded) electron-electron interaction  $D_0$ . The following proof is based on momentum conservation, thus it is a form of Ward identity. We use the perturbative expansion; the validity of the proof, however, is not restricted to any finite order of diagrams. All Green's functions in this appendix are the causal functions at zero temperature.

We assume that the polarization operator  $\Pi$  is a functional of the bare electron Green's functions  $G_0$  and the bare boson Green's function  $D_0$ . This assumption allows us to perform the derivative  $\partial/\partial A$  explicitly. At zero temperature the bare electron Green's function is [see Ref. 8, Eq. (7.7)]

$$G_0(k, z) = \frac{1}{z - \epsilon_{k-eA} + i\delta_k}, \quad (\text{B1})$$

where  $\delta_k$  is an infinitesimal function positive above the Fermi level and negative below. From (B1), one can check the basic relation for the Ward identity

$$\frac{\partial G_0(k, z)}{\partial A} = \frac{e}{m} k \frac{\partial G_0(k, z)}{\partial z}, \quad (\text{B2})$$

which will help to prove (51) for a general diagram.

### 1. Derivative of individual diagrams of $\Pi$

Assume that the polarization operator is expressed as the sum of diagrams

$$\Pi(q, \omega) = \sum_C \eta^C \Pi^C(q, \omega), \quad (\text{B3})$$

where  $\eta^C$  is a factor of the diagram  $C$  given by its order  $n^C$  and its number of closed loops. The diagram  $C$  has a form

$$\begin{aligned} \Pi^C(q, \omega) &= \int \prod_{j=1}^{n^C} \frac{dE_j}{2\pi} \frac{dp_j}{(2\pi)^d} \prod_{m=1}^{n^C-1} D_0(q_m, \omega_m) \\ &\quad \times \prod_{n=1}^{2n^C} G_0(k_n, z_n), \end{aligned} \quad (\text{B4})$$

where the multiple products relate only to functions having the product index as an explicit argument. According to general rules (see Ref. 8, Chap. II), the diagram  $C$  has  $n^C - 1$  bare boson lines  $D_0$ ,  $2n^C$  bare electron lines  $G_0$ , and  $2n^C$  vertices. Each line brings a new pair of variables  $(k, z)$  and each vertex brings a momentum and energy conserving  $\delta$  function. Two external vertices couple internal variables to the momentum-energy argument  $(q, \omega)$ . One ends up with  $n^C$  independent internal variables  $(p_j, E_j)$  and one external variable  $(q, \omega)$ . The arguments of the Green's functions are linear combinations of the independent variables

$$(k_n, z_n) = (q, \omega) \eta_n^C + \sum_{j=1}^{n^C} (p_j, E_j) \eta_{nj}^C. \quad (\text{B5})$$

The arguments of the bare boson lines  $(q_m, \omega_m)$  are given by a similar linear combination. We will not need them, however, in the explicit form.

According to (B5) the product  $k\partial/\partial z$  from (B2) can be rearranged as

$$k_n \frac{\partial}{\partial z_n} G_0(k_n, z_n) = \left( q \frac{\partial}{\partial \omega} + \sum_{j=1}^{n^C} p_j \frac{\partial}{\partial E_j} \right) G_0(k_n, z_n). \quad (\text{B6})$$

The right-hand side of (B6) has the advantage that a single differential operator applies to all lines of a given diagram. According to (B6)

$$\begin{aligned} \frac{\partial \Pi^C(q, \omega)}{\partial A} &= \frac{e}{m} \int \prod_{j=1}^{n^C} \frac{dE_j}{2\pi} \frac{dp_j}{(2\pi)^d} \prod_{m=1}^{n^C-1} D_0(q_m, \omega_m) \\ &\quad \times \left( q \frac{\partial}{\partial \omega} + \sum_{j=1}^{n^C} p_j \frac{\partial}{\partial E_j} \right) \prod_{n=1}^{2n^C} G_0(k_n, z_n). \end{aligned} \quad (\text{B7})$$

### 2. Instant potential approximation

All the derivatives apply only to bare electron lines. We use the simple identity  $D\partial G = \partial(DG) - G\partial D$  to rearrange (B7) as

$$\begin{aligned} \frac{\partial \Pi^C(q, \omega)}{\partial A} &= \frac{e}{m} \int \prod_{j=1}^{n^C} \frac{dE_j}{2\pi} \frac{dp_j}{(2\pi)^d} \left( q \frac{\partial}{\partial \omega} + \sum_{j=1}^{n^C} p_j \frac{\partial}{\partial E_j} \right) \\ &\quad \times \prod_{m=1}^{n^C-1} D_0(q_m, \omega_m) \prod_{n=1}^{2n^C} G_0(k_n, z_n) \\ &\quad - \frac{e}{m} \int \prod_{j=1}^{n^C} \frac{dE_j}{2\pi} \frac{dp_j}{(2\pi)^d} \prod_{n=1}^{2n^C} G_0(k_n, z_n) \\ &\quad \times \left( q \frac{\partial}{\partial \omega} + \sum_{j=1}^{n^C} p_j \frac{\partial}{\partial E_j} \right) \prod_{m=1}^{n^C-1} D_0(q_m, \omega_m). \end{aligned} \quad (\text{B8})$$

In the first term we use integration by parts to eliminate all derivatives with respect to  $E_j$ . The only nonzero contribution of the first term is therefore proportional to  $q\partial/\partial\omega$ ; this operator can be interchanged with the integrations and the integrand becomes identical to  $\Pi^C$  in (B6). Thus

$$\begin{aligned} \frac{\partial\Pi^C(q,\omega)}{\partial A} &= \frac{e}{m}q\frac{\partial}{\partial\omega}\Pi^C(q,\omega) \\ &\quad - \frac{e}{m}\int\prod_{j=1}^{n^c}\frac{dE_j}{2\pi}\frac{dp_j}{(2\pi)^d}\prod_{n=1}^{2n^c}G_0(k_n,z_n) \\ &\quad \times\left(q\frac{\partial}{\partial\omega}+\sum_{j=1}^{n^c}p_j\frac{\partial}{\partial E_j}\right)\prod_{m=1}^{n^c-1}D_0(q_m,\omega_m). \end{aligned} \quad (\text{B9})$$

The first term is the desirable energy derivative of the polarization operator. Indeed, summing over all diagrams, one recovers formula (51). The second term in (B9) is a correction which is zero in two important cases: first, for instant (i.e., energy-independent) bare boson lines and second, within the RPA of the polarization operator. We are not in a position to give any estimation of this correction; however, we believe that formula (51) might be a good approximation for a wide class of systems. In the case of the retarded bare boson lines we want to call formula (51) the instant potential approximation.

### APPENDIX C: BACK FLOW OF WAVES AND BOSONS UNIFIED

In this appendix we prove that the wave back flow of bosons can be evaluated as a quadratic response where the fluctuations of the internal field equal to  $\phi^{(2)}$  are given by (55). Although microscopic mechanisms of the wave back flow of bosons are identical to the quadratic response, these two problems have quite different boundary conditions. The response starts from the ground state and the current appears as the system is driven out of the ground state by the external field. In contrast, the nonequilibrium distribution of bosons is a part of the initial condition and the system is in a steady state. Accordingly, we need a different approach based on nonequilibrium Green's functions.

#### 1. Current in terms of functional derivatives

Within the Kadanoff-Baym formalism, the homogeneous electric current reads

$$j(t_0) = e\int\frac{dk}{(2\pi)^d}\frac{\partial\epsilon_k}{\partial k}i\Delta G(t_0,t_0^+,k), \quad (\text{C1})$$

where  $\epsilon_k$  is the bare electron dispersion relation and  $\Delta G$  is the deviation of the nonequilibrium single-electron Green's function from equilibrium. This function is defined with the help of a time ordering on a closed time path (see Ref. 9 or Appendix A), and  $t_0^+$  stands in the

time ordering after  $t_0$ , although it has the same value.

We resume a diagrammatic expansion of  $G$  only along boson lines. Thus we take the single-electron Green's function as a functional  $G[G_0,D]$ . This choice of the functional simplifies an expansion in the perturbation  $\Delta D$ ; in particular we can write

$$\Delta G(t_0,t_0^+;k) = \Delta D(\bar{1},\bar{2})\frac{\delta G(t_0,t_0^+;k)}{\delta D(\bar{1},\bar{2})}, \quad (\text{C2})$$

because the boson distribution does not affect the free-electron Green's function  $G_0$ .

The current  $j(t_0)$  is a linear combination of elements  $G(t_0,t_0^+;k)$ . This linear combination can be interchanged with the functional derivative which emerges in (C2); thus

$$j(t_0) = \Delta D(\bar{1},\bar{2})\frac{\delta}{\delta D(\bar{1},\bar{2})}e\int\frac{dk}{(2\pi)^d}\frac{\partial\epsilon_k}{\partial k}G(t_0,t_0^+,k). \quad (\text{C3})$$

In Eq. (C3) the  $\Delta G(t_0,t_0^+;k)$  is expressed in terms of the functional derivative of the equilibrium single-electron Green's function  $G(t_0,t_0^+;k)$ . We can use an equilibrium generating functional  $L$  [see Eq. (A4)] to generate the linear combination giving the current by the functional derivative with respect to a vector potential  $A$

$$j(t_0) = \frac{1}{\Omega}\Delta D(\bar{1},\bar{2})\frac{\delta}{\delta D(\bar{1},\bar{2})}\frac{\delta L}{\delta A(t_0)}. \quad (\text{C4})$$

#### 2. Full potential-potential correlator $\Delta D$

Now we find  $\Delta D$ . For free bosons, the deviation of the boson Green's function is given by (54), but in the interacting system, formula (54) covers only a change of the boson Green's function at singularities. There are also changes of the regular part of the boson Green's function  $D$  resulting from the effect of the bosons on the electron subsystem and via the polarization operator  $\Pi$  projected back in  $D$ . Within the linear approximation in the boson distribution, the total change of the boson Green's function is given by

$$\Delta D(1,2) = -i\phi^{(2)}(1,2) + \Delta D(\bar{5},\bar{6})\frac{\delta\Pi(\bar{3},\bar{4})}{\delta D(\bar{5},\bar{6})}\frac{\delta D(1,2)}{\delta\Pi(\bar{3},\bar{4})}, \quad (\text{C5})$$

where  $\phi^{(2)}$  is defined by (55). The functional derivatives in (C5) have the following meaning. From the dressing of the boson Green's function  $D^{-1} = D_0^{-1} - \Pi$ , one finds  $\delta D(1,2)/\delta\Pi(3,4) = D(1,3)D(4,2)$ . The polarization operator  $\Pi$  in the functional derivative is a functional of the dressed boson and the bare electron Green's function  $\Pi[G_0,D]$ .

We denote the formal solution of (C5) by

$$\Delta D(1,2) = -i\phi^{(2)}(\bar{3},\bar{4})M(\bar{3},\bar{4};1,2), \quad (\text{C6})$$

where  $M$  is a four-argument function obtained by iter-

ation of (C5). Therefore, the current depends on  $\phi^{(2)}$  as

$$j(t_0) = -\frac{i}{\Omega} \phi^{(2)}(\bar{1}, \bar{2}) M(\bar{1}, \bar{2}; \bar{3}, \bar{4}), \frac{\delta}{\delta D(\bar{3}, \bar{4})} \frac{\delta L}{\delta A(t_0)}. \quad (C7)$$

### 3. Independent variational fields

The basic trick that allowed us to develop the quadratic response theory of the wave back flow in terms of the linear response was to take the functional derivative with respect to the vector potential as the last one. In contrast to the quadratic response, in (C4) the order of the two derivatives cannot be interchanged because the dressed boson Green's function  $D$  depends on a motion of electrons, i.e., the two derivatives are not independent.

Fortunately, we can rearrange (C4) in terms of functional derivatives with respect to an independent field  $\delta D_0$ , which is a trial double-time function added to the true bare boson Green's function. Using a composed derivative

$$\frac{\delta}{\delta D_0(1, 2)} = \frac{\delta D(\bar{3}, \bar{4})}{\delta D_0(1, 2)} \frac{\delta}{\delta D(\bar{3}, \bar{4})}, \quad (C8)$$

we obtain  $\delta/\delta D$ , needed in (C4) in terms of  $\delta/\delta D_0$ .

Before we substitute  $\delta/\delta D$  from (C8) into (C4) it is advantageous to rearrange  $\delta D/\delta D_0$ . From  $D^{-1} = D_0^{-1} - \Pi$  one finds

$$\frac{\delta D(3, 4)}{\delta D_0(1, 2)} = \varepsilon^{-1}(3, 1) \varepsilon^{-1}(4, 2) + \frac{\delta \Pi(\bar{5}, \bar{6})}{\delta D_0(1, 2)} \frac{\delta D(3, 4)}{\delta \Pi(\bar{5}, \bar{6})}. \quad (C9)$$

Writing the derivative of  $\Pi$  as composed we find

$$\begin{aligned} \frac{\delta D(3, 4)}{\delta D_0(1, 2)} &= \frac{\delta D(\bar{7}, \bar{8})}{\delta D_0(1, 2)} \frac{\delta \Pi(\bar{5}, \bar{6})}{\delta D(\bar{7}, \bar{8})} \frac{\delta D(3, 4)}{\delta \Pi(\bar{5}, \bar{6})} \\ &= \varepsilon^{-1}(3, 1) \varepsilon^{-1}(4, 2). \quad (C10) \end{aligned}$$

Comparing (C10) with (C5) one observes that "coefficients of the linear combination" on both left-hand sides

are identical, therefore

$$\frac{\delta D(3, 4)}{\delta D_0(1, 2)} = \varepsilon^{-1}(\bar{5}, 1) \varepsilon^{-1}(\bar{6}, 2) M(\bar{5}, \bar{6}; 3, 4). \quad (C11)$$

According to (C11) the operator needed in (C7) can be written as

$$M(1, 2; \bar{3}, \bar{4}) \frac{\delta}{\delta D(\bar{3}, \bar{4})} = \varepsilon(\bar{3}, 1) \varepsilon(\bar{4}, 2) \frac{\delta}{\delta D_0(\bar{3}, \bar{4})}. \quad (C12)$$

### 4. Relation to the quadratic response

The functional derivative with respect to  $\delta D_0$  is only a tool which generates two pairs of the local density operators for prescribed arguments. Thus it can be replaced by two functional derivatives with respect to an external field  $\delta\varphi$ ,

$$\frac{\delta}{\delta D_0(1, 2)} = \frac{i}{2} \frac{\delta^2}{\delta\varphi(2)\delta\varphi(1)}. \quad (C13)$$

The factor 1/2 comes with two-particle potentials into the Hamiltonian [see Ref. 8, Eq. (6.4)]. The complex unit compensates an exceeding 1/ $i$  emerging with each order of the functional derivative.

Now we are ready to express the wave back flow of bosons using formulas for the quadratic response. We use (C12) and (C13) in (C7) to obtain

$$j(t_0) = \frac{1}{2\Omega} \phi^{(2)}(\bar{1}, \bar{2}) \varepsilon(\bar{3}, \bar{1}) \varepsilon(\bar{4}, \bar{2}) \frac{\delta^2}{\delta\varphi(\bar{4})\delta\varphi(\bar{3})} \frac{\delta L}{\delta A(t_0)}. \quad (C14)$$

This equation already belongs to the family of the quadratic response theory treated in Appendix A. We interchange the order of derivatives and use (A9)

$$j(t_0) = \frac{1}{2\Omega} \phi^{(2)}(\bar{1}, \bar{2}) \frac{\delta \Pi(\bar{1}, \bar{2})}{\delta A(t_0)}. \quad (C15)$$

This formula is equivalent to (A14); therefore the boson back flow obtained from the quadratic response using  $\phi^{(2)}$  as the square of the internal field is an exact result.

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