Extension of the Kubo formula for the electrical-conductivity tensor to arbitrary polarizations of the electric field

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It is shown that there are two different electrical-conductivity tensors which may be defined naturally by the relation $\mathbf{J}=\vec{\sigma}\cdot\mathbf{E}$. The $\vec{\sigma}_{\rm Kubo}$ given by the standard Kubo formula is different, in general, from the $\vec{\sigma}_{\rm max}$ appearing in Maxwell's equations, although they do agree if the electric field is transverse ($\mathbf{q}\cdot\mathbf{E}=0$). It is also shown how the Kubo formula may be modified to give $\vec{\sigma}_{\rm max}$ when the field is not transverse.

I. INTRODUCTION

Consider a material in the presence of an electric field (in the long-wavelength limit)

$$\mathbf{E}(\mathbf{x},t)=\mathbf{E}_0 e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}e^{\eta t}\ , \tag{1.1}$$

where η is a positive infinitesimal to turn on the field adiabatically from time $t=-\infty$. The Fourier transform of the ensemble average of the resulting current density is given by (to first order in E_0)

$$J_\alpha(\mathbf{q}',\omega')=\delta_{\mathbf{q}',\mathbf{q}}\delta(\omega'-\omega)\sum_\beta \sigma_{\alpha\beta}(\mathbf{q},\omega)E_{0\beta}\ , \tag{1.2}$$

where $\sigma_{\alpha\beta}(\mathbf{q},\omega)$ is the frequency- and wave-vector-dependent electrical-conductivity tensor (α and β are coordinate indices). This conductivity tensor is then given by the well-known Kubo formula[1]

$$\sigma_{\alpha\beta}(\mathbf{q},\omega)=-\frac{1}{\hbar\omega}\int_{-\infty}^{0}d\tau\, e^{-i(\omega+i\eta)\tau}\times\langle[J_\beta(\mathbf{q},\tau),J_\alpha(\mathbf{q},0)]\rangle\ , \tag{1.3}$$

where the square brackets denote a commutator, and the angular brackets denote an ensemble average in the absence of the electric field. Here $\mathbf{J}(\mathbf{q},\tau)$ is the Heisenberg operator

$$\mathbf{J}(\mathbf{q},\tau)=e^{i\hbar^{-1}H_0\tau}\mathbf{J}(\mathbf{q})e^{-i\hbar^{-1}H_0\tau}\ , \tag{1.4}$$

with H_0 the Hamiltonian of the system in the absence of the field. This Kubo formula is discussed in more detail in the next section.

In this paper it will be shown that the conductivity tensor given by this formula is not, in general, the same as that appearing in Maxwell's equations[2]

$$\nabla\times\mathbf{B}-\frac{1}{c}\frac{\partial\mathbf{E}}{\partial t}=\frac{4\pi}{c}(\mathbf{J}_{\rm ext}+\mathbf{J}_{\rm int})\ ,$$

or

$$i\mathbf{q}\times\mathbf{B}+\frac{i\omega}{c}\mathbf{E}=\frac{4\pi}{c}(\mathbf{J}_{\rm ext}+\vec{\sigma}\cdot\mathbf{E}) \tag{1.5}$$

(when coordinate indices are not used explicitly, tensors will be indicated with an overhead, double-ended arrow). In the remainder of this paper, these two conductivities will be referred to as the Kubo conductivity $\vec{\sigma}_{\rm Kubo}$ and the Maxwell conductivity $\vec{\sigma}_{\rm max}$, respectively. It will also be shown how the Kubo formula may be modified to give $\vec{\sigma}_{\rm max}$. Finally, we will see that, for transverse fields ($\mathbf{q}\cdot\mathbf{E}_0=0$), which is the case in which the Kubo formula is generally used, $\vec{\sigma}_{\rm Kubo}=\vec{\sigma}_{\rm max}$. Thus, this modified formula for $\vec{\sigma}_{\rm max}$ may be viewed as an extension of the Kubo formula from transverse fields to fields of arbitrary polarization.

There has been some previous work along these lines. Kubo himself was aware of this difference, and, for longitudinal fields, he showed[3] that $\vec{\sigma}_{\rm max}$ is given by

$$\vec{\sigma}_{\rm max}(\mathbf{q},\omega)=\left[1-\frac{i4\pi}{\omega}\hat{\mathbf{q}}\cdot\vec{\sigma}_{\rm Kubo}(\mathbf{q},\omega)\cdot\hat{\mathbf{q}}\right]^{-1}\times\vec{\sigma}_{\rm Kubo}(\mathbf{q},\omega)\ , \tag{1.6}$$

where $\hat{\mathbf{q}}$ denotes a unit vector along $\mathbf{q}$. Even earlier, for cubic crystals, Ambegaokar and Kohn[4] obtained results very similar to the ones presented in this paper. However, they included only the electronic contribution to the conductivity, and they relied heavily on the fact that, for cubic materials in the long-wavelength limit, the conductivity tensor must have the special form

$$\sigma_{\alpha\beta}(\mathbf{q},\omega)=\delta_{\alpha\beta}\sigma^{(1)}(\omega)+\hat{q}_\alpha\hat{q}_\beta\sigma^{(2)}(\omega)\ , \tag{1.7}$$

where $\sigma^{(1)}(\omega)$ and $\sigma^{(2)}(\omega)$ are scalar functions. The results presented in this paper will include the contributions from all of the charge species, including the ions, and they will be valid for conductivity tensors of any form (i.e., for crystals of any symmetry).

Also, note that, for the special form (1.7), the conductivities for transverse and longitudinal fields are given, respectively, by the scalar quantities

$$\sigma^{(\rm T)}(\omega)=\sigma^{(1)}(\omega)\ , \tag{1.8}$$

$$\sigma^{(\rm L)}(\omega)=\sigma^{(1)}(\omega)+\sigma^{(2)}(\omega)\ . \tag{1.9}$$

Therefore, in this case, one can construct the tensor $\vec{\sigma}_{\rm max}$

for fields of arbitrary polarization from a knowledge of $\vec{\sigma}_{\text{Kubo}}$ using only the simple relations already mentioned:

$$\sigma^{(\text{T})}_{\text{max}}(\omega)=\sigma^{(\text{T})}_{\text{Kubo}}(\omega)\ , \tag{1.10}$$

$$\sigma^{(\text{L})}_{\text{max}}(\omega)=\left[1-\frac{i4\pi}{\omega}\sigma^{(\text{L})}_{\text{Kubo}}(\omega)\right]^{-1}\sigma^{(\text{L})}_{\text{Kubo}}(\omega)\ . \tag{1.11}$$

However, we will see that it is easier to find $\sigma^{(\text{L})}_{\text{max}}(\omega)$ directly than to find $\sigma^{(\text{L})}_{\text{Kubo}}(\omega)$ in the first place (this is true for both this paper and that of Ambegaokar and Kohn).

II. KUBO FORMULA

In this section a brief discussion of the Kubo formula is given. Consider a system with Hamiltonian

$$H(t)=H_0+V(t)\ , \tag{2.1}$$

where the perturbation $V(t)$ has the form

$$V(t)=V_0e^{-i\omega t}e^{\eta t}\ . \tag{2.2}$$

To first order in this perturbation, the change in the ensemble average of an operator Γ is given by the linear-response function[1]

$$\Gamma_1(t)=e^{-i(\omega+i\eta)t}\Gamma'(\omega)\ , \tag{2.3}$$

where

$$\Gamma'(\omega)=\frac{i}{\hbar}\int_{-\infty}^{0}d\tau e^{-i(\omega+i\eta)\tau}\langle[V_0(\tau),\Gamma]\rangle\ , \tag{2.4}$$

with $V_0(\tau)$ being the Heisenberg operator

$$V_0(\tau)=e^{i\hbar^{-1}H_0\tau}V_0e^{-i\hbar^{-1}H_0\tau}\ . \tag{2.5}$$

The angular brackets in (2.4) denote an ensemble average in the absence of the perturbation $V(t)$.

It will now be shown how Eq. (1.3) follows from this. A gauge may be chosen with

$$\phi(\mathbf{x},t)=0\ , \tag{2.6}$$

$$\mathbf{A}(\mathbf{x},t)=\mathbf{A}_0e^{i(\mathbf{q}\cdot\mathbf{x}-\omega t)}e^{\eta t}\ . \tag{2.7}$$

The perturbation is then given by

$$V(t)=-\frac{1}{c}\int d^3x\,\mathbf{J}\cdot\mathbf{A}=V_0e^{-i\omega t}e^{\eta t}\ , \tag{2.8}$$

with c denoting the speed of light and

$$V_0=-\frac{1}{c}\mathbf{J}(\mathbf{q})\cdot\mathbf{A}_0=\frac{i}{\omega}\sum_{\beta}J_\beta(\mathbf{q})E_{0\beta}\ , \tag{2.9}$$

where use has been made of $\mathbf{E}=-c^{-1}\partial\mathbf{A}/\partial t=i\omega c^{-1}\mathbf{A}$ to relate $\mathbf{A}_0$ and $\mathbf{E}_0$. Using (2.9) in (2.3) and (2.4) with $\Gamma=J_\alpha$ and then Fourier transforming yields (1.3). The important thing to note here is that the electric field appearing in the perturbation (2.8) and (2.9) is the field that appears in Eq. (1.2). We will see in the next section that this point is very important.

Finally, let me comment that, for simplicity, this paper deals with the canonical ensemble. However, all of the results presented here are also valid for the grand canonical ensemble if Eq. (1.4) is replaced by

$$\mathbf{J}(\mathbf{q},\tau)=e^{i\hbar^{-1}\Omega_0\tau}\mathbf{J}(\mathbf{q})e^{-i\hbar^{-1}\Omega_0\tau}\ , \tag{2.10}$$

where $\Omega_0=H_0-\mu N$ is the grand potential.

III. EXTERNAL AND LOCAL CONDUCTIVITIES

There are two different electrical conductivity tensors which may be defined naturally by the relation

$$\mathbf{J}=\vec{\sigma}\cdot\mathbf{E}\ , \tag{3.1}$$

depending on whether $\mathbf{E}$ is the applied field or the local (screened) field. Kubo[3] has called these the external and local conductivities, respectively:

$$\mathbf{J}=\vec{\sigma}_{\text{ext}}\cdot\mathbf{E}_{\text{app}} \tag{3.2}$$

$$=\vec{\sigma}_{\text{loc}}\cdot\mathbf{E}_{\text{loc}}\ . \tag{3.3}$$

Since Maxwell's equations involve the local fields, then the Maxwell conductivity is the local conductivity $\vec{\sigma}_{\text{max}}=\vec{\sigma}_{\text{loc}}$.

In Sec. II it was shown that the electric field which appears in Eq. (1.2) is the one which appears in the perturbation (2.8) and (2.9). The Hamiltonian was written as

$$H(t)=H_0+V(t)\ , \tag{3.4}$$

$$V(t)=-\frac{1}{c}\int d^3x\,\mathbf{J}\cdot\mathbf{A}\ , \tag{3.5}$$

where H_0 is the Hamiltonian in the absence of the field. Thus, H_0 contains all of the interactions which screen the field (e.g., Coulomb interactions between electrons), so that the perturbation must contain only the unscreened (applied) field $\mathbf{E}_{\text{app}}$. Therefore, the Kubo conductivity is the external conductivity $\vec{\sigma}_{\text{Kubo}}=\vec{\sigma}_{\text{ext}}$.

We now see why the Kubo and Maxwell conductivities differ in general. It is also clear why they agree for transverse fields, since, for such fields, screening does not occur,[5] so that $\mathbf{E}_{\text{loc}}=\mathbf{E}_{\text{app}}$ and $\vec{\sigma}_{\text{loc}}=\vec{\sigma}_{\text{ext}}$. In addition, we can now see how to modify the Kubo formula to give the Maxwell conductivity $\vec{\sigma}_{\text{max}}=\vec{\sigma}_{\text{loc}}$. What we need to write is

$$H(t)=\tilde{H}_0+\tilde{V}(t)\ , \tag{3.6}$$

$$\tilde{V}(t)=-\frac{1}{c}\int d^3x\,\mathbf{J}\cdot\mathbf{A}_{\text{loc}}\ . \tag{3.7}$$

Then (1.3) will give $\vec{\sigma}_{\text{max}}$ when the ensemble average is taken for a system with Hamiltonian $\tilde{H}_0$. However, $\tilde{H}_0$ is just H_0 with all of the long-range (screening) interactions removed (this will be shown more explicitly in the next section). Therefore, in evaluating (1.3), simply leave out all Feynman diagrams which contain long-range interactions (this statement is made more precise in Sec. V).

Finally, we can now see why less work is involved in finding $\vec{\sigma}_{\text{max}}$ than in finding $\vec{\sigma}_{\text{Kubo}}$, since the former involves summing only a subset of the diagrams appearing in the latter.

IV. RELATING $\vec{\sigma}_{\text{Kubo}}$ AND $\vec{\sigma}_{\text{max}}$

In this section it will be shown explicitly that evaluating $\vec{\sigma}_{\text{Kubo}}$ with all long-range interactions removed from

the unperturbed Hamiltonian does indeed yield $\overleftrightarrow{\sigma}_{\max}$ (in the next section it is shown how this is done in practice). We may write

$$\mathbf{E}_{\rm loc}=\mathbf{E}_{\rm app}+\mathbf{E}_{\rm scr} , \tag{4.1}$$

where $\mathbf{E}_{\rm scr}$ is the screening field set up by the interactions in H_0. Let the part of H_0 which contributes to $\mathbf{E}_{\rm scr}$ be denoted by $H_{\rm LR}$ (these are the long-range interactions), and let the remainder of H_0 be denoted by $H_{\rm SR}$ (these are the short-range interactions).[6] This yields

$$H=H_0+V=H_{\rm SR}+H_{\rm LR}+V , \tag{4.2}$$

where V contains only the applied field $\mathbf{E}_{\rm app}$.

Now, the material consists of electrons and ions. For the sake of clarity, the ions will be treated classically with the displacement of the ith ion from equilibrium being denoted by $\mathbf{u}_i$. However, this approximation is not necessary, and the ions can be given a rigorous quantum-mechanical treatment (I will return to this point at the end of this section). The electrons will be given a rigorous quantum-mechanical treatment using the equations of motion for the expectation values of the position and momentum operators of the jth electron:

$$\frac{d}{dt}\langle \mathbf{x}_j\rangle=\frac{1}{m}\langle \mathbf{p}_j\rangle , \tag{4.3}$$

$$\frac{d}{dt}\langle \mathbf{p}_j\rangle=-\left\langle\frac{\partial H}{\partial \mathbf{x}_j}\right\rangle , \tag{4.4}$$

where m is the electron mass. Here, care must be taken since the quantity $\langle \mathbf{x}_j\rangle$ is not well defined in the limit of infinite volume. Thus, I will begin by considering a material of of finite volume Ω, for which $\langle \mathbf{x}_j\rangle$ is well defined. However, the final results will not involve $\langle \mathbf{x}_j\rangle$, so, at that point, we may let $\Omega\rightarrow\infty$ if we wish.

The force on the ith ion is given by

$$\mathbf{F}_i=-\frac{\partial H}{\partial \mathbf{u}_i} . \tag{4.5}$$

However, by construction,

$$-\frac{\partial H_{\rm LR}}{\partial \mathbf{u}_i}=e_i\mathbf{E}_{\rm scr} , \tag{4.6}$$

$$-\frac{\partial V}{\partial \mathbf{u}_i}=e_i\mathbf{E}_{\rm app} , \tag{4.7}$$

where e_i is the charge of the ith ion, so that

$$\mathbf{F}_i=-\frac{\partial H_{\rm SR}}{\partial \mathbf{u}_i}+e_i\mathbf{E}_{\rm loc} , \tag{4.8}$$

which yields an equation of motion for $\mathbf{u}_i$:

$$\frac{M_i}{e_i}\frac{d^2}{dt^2}\mathbf{u}_i+\frac{1}{e_i}\frac{\partial H_{\rm SR}}{\partial \mathbf{u}_i}=\mathbf{E}_{\rm loc} , \tag{4.9}$$

where M_i is the mass of the ith ion.

Since we know that the ion positions $\mathbf{u}_i$ are well defined, then this equation must have a solution, which will be denoted by

$$\mathbf{u}_i=\mathbf{g}_i(\mathbf{E}_{\rm loc}) . \tag{4.10}$$

The important thing to notice here is that the form of the function $\mathbf{g}_i$ depends only on the left-hand side of (4.9). The right-hand side of (4.9) affects only the argument of $\mathbf{g}_i$. Therefore, if $H_{\rm LR}$ is removed from H_0, a similar computation yields

$$\frac{M_i}{e_i}\frac{d^2}{dt^2}\mathbf{u}_i+\frac{1}{e_i}\frac{\partial H_{\rm SR}}{\partial \mathbf{u}_i}=\mathbf{E}_{\rm app} , \tag{4.11}$$

for which the solution must be

$$\mathbf{u}_i'=\mathbf{g}_i(\mathbf{E}_{\rm app}) , \tag{4.12}$$

with the same function $\mathbf{g}_i$ as in (4.10) (in this section, primes will be used to label quantities in the case where $H_{\rm LR}$ has been removed from H_0).

The electrons are now handled similarly using Eqs. (4.3) and (4.4). By construction,

$$-\left\langle\frac{\partial H_{\rm LR}}{\partial \mathbf{x}_j}\right\rangle=-e\mathbf{E}_{\rm scr} , \tag{4.13}$$

$$-\left\langle\frac{\partial V}{\partial \mathbf{x}_j}\right\rangle=-e\mathbf{E}_{\rm app} , \tag{4.14}$$

where $-e$ is the electron charge, so that

$$\frac{d^2}{dt^2}\langle \mathbf{x}_j\rangle=\frac{1}{m}\frac{d}{dt}\langle \mathbf{p}_j\rangle=-\frac{1}{m}\left\langle\frac{\partial H}{\partial \mathbf{x}_j}\right\rangle ,$$

or

$$-\frac{m}{e}\frac{d^2}{dt^2}\langle \mathbf{x}_j\rangle-\frac{1}{e}\left\langle\frac{\partial H_{\rm SR}}{\partial \mathbf{x}_j}\right\rangle=\mathbf{E}_{\rm loc} . \tag{4.15}$$

Again, we know that $\langle \mathbf{x}_j\rangle$ is well defined, so that this equation must have a solution, which will be denoted by

$$\langle \mathbf{x}_j\rangle=\mathbf{G}_j(\mathbf{E}_{\rm loc}) , \tag{4.16}$$

where, again, the form of the function $\mathbf{G}_j$ depends only on the left-hand side of (4.15). Therefore, if $H_{\rm LR}$ is removed from H_0, a similar computation yields

$$-\frac{m}{e}\frac{d^2}{dt^2}\langle \mathbf{x}_j\rangle-\frac{1}{e}\left\langle\frac{\partial H_{\rm SR}}{\partial \mathbf{x}_j}\right\rangle=\mathbf{E}_{\rm app} , \tag{4.17}$$

for which the solution must be

$$\langle \mathbf{x}_j\rangle'=\mathbf{G}_j(\mathbf{E}_{\rm app}) , \tag{4.18}$$

with the same function $\mathbf{G}_j$ as in (4.16).

Now, consider the electric polarization

$$\mathbf{P}=\frac{1}{\Omega}\left[\sum_j(-e\langle \mathbf{x}_j\rangle)+\sum_i e_i\mathbf{u}_i\right] . \tag{4.19}$$

With $H_{\rm LR}$ present, this is given by

$$\mathbf{P}=\frac{1}{\Omega}\left[-e\sum_j\mathbf{G}_j(\mathbf{E}_{\rm loc})+\sum_i e_i\mathbf{g}_i(\mathbf{E}_{\rm loc})\right] . \tag{4.20}$$

To first order in $\mathbf{E}_{\rm loc}$, this must be

$$\mathbf{P}=\overleftrightarrow{\chi}\cdot\mathbf{E}_{\rm loc} , \tag{4.21}$$

where $\overleftrightarrow{\chi}$ is the (Maxwell) electric susceptibility tensor of the material.

Since $\vec{\vec{\chi}}$ is independent of $\mathbf{E}_{\rm loc}$,[7] its value must depend only on the forms of the functions $\mathbf{G}_j$ and $\mathbf{g}_i$ [remember that Eqs. (4.20) and (4.21) are valid for any value of the field $\mathbf{E}_{\rm loc}$, so that their equivalence is an equivalence of functions]. Therefore, with $H_{\rm LR}$ absent, we must have

$$\mathbf{P}'=\frac{1}{\Omega}\left[\sum_j(-e\langle\mathbf{x}_j\rangle')+\sum_i e_i\mathbf{u}_i'\right]$$
$$=\frac{1}{\Omega}\left[-e\sum_j\mathbf{G}_j(\mathbf{E}_{\rm app})+\sum_i e_i\mathbf{g}_i(\mathbf{E}_{\rm app})\right]$$
$$=\vec{\vec{\chi}}\cdot\mathbf{E}_{\rm app}\,, \tag{4.22}$$

with the same value of $\vec{\vec{\chi}}$ as in (4.21). Since[8]

$$\vec{\vec{\sigma}}=-i\omega\vec{\vec{\chi}}\,, \tag{4.23}$$

Eq. (4.21) yields (with $H_{\rm LR}$ present)

$$\vec{\vec{\sigma}}_{\rm max}=-i\omega\vec{\vec{\chi}}\,, \tag{4.24}$$

while (4.22) yields (with $H_{\rm LR}$ absent)

$$\vec{\vec{\sigma}}'_{\rm Kubo}=-i\omega\vec{\vec{\chi}}\,. \tag{4.25}$$

Thus, $\vec{\vec{\sigma}}'_{\rm Kubo}=\vec{\vec{\sigma}}_{\rm max}$, which finally shows that the Kubo conductivity in the absence of $H_{\rm LR}$ equals the Maxwell conductivity in the presence of $H_{\rm LR}$, so that the Kubo formula (1.3) may be used to find the Maxwell conductivity $\vec{\vec{\sigma}}_{\rm max}$ if all long-range (screening) interactions are removed from the unperturbed Hamiltonian.

Let me now return to the comments made near the beginning of this section about the manner in which the ions are treated. The classical treatment of the ions which was presented served as a motivation for the rigorous treatment of the electrons. However, this latter treatment can be repeated for any charged particle (electron, lattice ion, impurity ion, etc.). For particle s, one obtains

$$\langle\mathbf{x}_s\rangle=\mathbf{G}_s(\mathbf{E}_{\rm loc})\,, \tag{4.26}$$

$$\langle\mathbf{x}_s\rangle'=\mathbf{G}_s(\mathbf{E}_{\rm app})\,, \tag{4.27}$$

where $\mathbf{x}_s$ denotes the position operator for particle s. Next, one obtains

$$\mathbf{P}=\frac{1}{\Omega}\sum_s e_s\langle\mathbf{x}_s\rangle$$
$$=\frac{1}{\Omega}\sum_s e_s\mathbf{G}_s(\mathbf{E}_{\rm loc})$$
$$=\vec{\vec{\chi}}\cdot\mathbf{E}_{\rm loc}\,, \tag{4.28}$$

$$\mathbf{P}'=\frac{1}{\Omega}\sum_s e_s\langle\mathbf{x}_s\rangle'$$
$$=\frac{1}{\Omega}\sum_s e_s\mathbf{G}_s(\mathbf{E}_{\rm app})$$
$$=\vec{\vec{\chi}}\cdot\mathbf{E}_{\rm app}\,, \tag{4.29}$$

where e_s is the charge of particle s. From here, the argument proceeds as before and yields the same result. Thus, we see that, as claimed, the ions can be treated rigorously without resorting to a classical treatment.

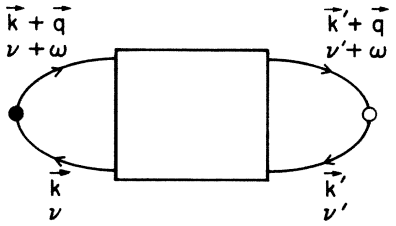

FIG. 1. General form of the diagrams contributing to (1.3). The solid lines are electrons, each of which is labeled by both a wave vector and a frequency, and the box represents any possible series of interactions (see Fig. 2). For $\vec{\sigma}(\mathbf{q},\omega)$, the solid (open) circle is a source (sink) of wave vector $\mathbf{q}$ and frequency ω.

V. FEYNMAN DIAGRAMS

In this section it will be stated more precisely what is meant by the removal of all long-range (screening) interactions from the unperturbed Hamiltonian, and this will indicate clearly which Feynman diagrams are to be omitted in the evaluation of $\vec{\vec{\sigma}}_{\rm max}$ from Eq. (1.3). Any interactions which screen the applied field must do so by coupling the electrons,[9] since they are the only mobile charge carriers. For simplicity, let us consider just one such interaction.

The Feynman diagrams which appear in (1.3) have the general form shown in Fig. 1. Specific examples of such diagrams are shown in Fig. 2. The problem which must be addressed is that of deciding which occurrences of the interaction in these diagrams contribute to the screening. Such a contribution must be long range, so that it must diverge as $q\to 0$. Of the diagrams in Fig. 2, only diagram (c) contains such a contribution,[10] since, as $q\to 0$, all other

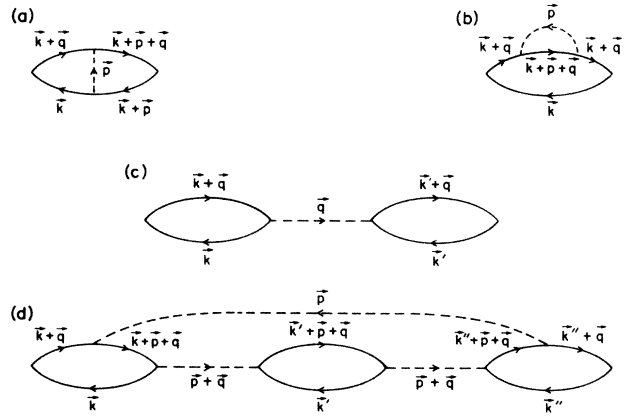

FIG. 2. Examples of diagrams contributing to (1.3). The solid lines are electrons, and the dashed lines are interactions between them (Coulomb interactions, phonons, etc.). Each line carries both wave vector and frequency, but, for simplicity, only the wave vectors are shown. Any wave vector other than $\mathbf{q}$ is integrated over.

occurrences of the interaction have finite wave vector $\mathbf{p}$ (which is integrated over). Thus, we see that not all occurrences of a long-range interaction contribute to the screening. While short-range interactions are entirely in H_{SR}, long-range interactions have parts in both H_{SR} and H_{LR},[11] and it is only these latter parts which are to be removed from H_0.

We can now see which diagrams are to be omitted from (1.3); they are just the diagrams which contain long-range interactions at the wave vector $\mathbf{q}$. However, these are just the improper[12] diagrams with respect to these interactions. This is easily seen by noticing (see Fig. 1) that the wave vector $\mathbf{q}$ flows through each diagram from left to right. Whenever there are two or more parallel channels for this flow, there will be an arbitrary division of the wave vector $\mathbf{q}$ between them (leading to one free wave vector per extra channel to be integrated over), so that no channel will be forced to have wave vector $\mathbf{q}$. Conversely, if removing a single interaction line leaves two disconnected pieces, then this line must be carrying the wave vector $\mathbf{q}$ from one piece to the other. Thus, the interaction lines at wave vector $\mathbf{q}$ are exactly those which make diagrams improper.

It is now possible to restate the modification of the Kubo formula more precisely. To use this formula to compute the Maxwell conductivity $\vec{\sigma}_{max}$, simply omit all Feynman diagrams which are improper with respect to a long-range interaction. Notice that, for a transverse field ($\mathbf{q}\cdot\mathbf{E}_0=0$), all interactions at wave vector $\mathbf{q}$ must also be transverse, so that all diagrams will already be proper with respect to all longitudinal interactions. Since long-range interactions are longitudinal, then the modification of the Kubo formula has no effect in this case. Thus, we again see that $\vec{\sigma}_{Kubo}=\vec{\sigma}_{max}$ for transverse fields.

The idea of retaining only the proper diagrams is not entirely new. As an example, Izuyama[13] has obtained the same result for metals. However, as in Ref. 4, only the electron contribution to the conductivity was considered, so that the only long-range interaction was the Coulomb interaction between electrons. In addition, Izuyama considered the case of a purely longitudinal electric field, leading to the same results obtained later (and more generally) by Kubo.[3] The point of the present paper is that these results can be extended to systems with many long-range interactions, including long-range interactions between different charge species. In a separate publication,[14] this formalism has been applied to a doped, polar semiconductor. There, in addition to the Coulomb interaction between electrons, one has the long-range Fröhlich interaction between the electrons and phonons (which arises from the Coulomb interaction between the electrons and ions). In this case, one must omit all diagrams which are improper with respect to either of these two interactions.

VI. CONCLUSIONS

There are two different electrical conductivities which may be defined naturally by the relation $\mathbf{J}=\vec{\sigma}\cdot\mathbf{E}$, depending on whether $\mathbf{E}$ is the applied field $\mathbf{E}_{app}$ or the local field $\mathbf{E}_{loc}$:

$$\mathbf{J}=\vec{\sigma}_{Kubo}\cdot\mathbf{E}_{app} \tag{6.1}$$

$$=\vec{\sigma}_{max}\cdot\mathbf{E}_{loc}\ . \tag{6.2}$$

In general, the Kubo formula for the conductivity yields $\vec{\sigma}_{Kubo}$. However, it has been shown that simply omitting all diagrams from this formula which are improper with respect to a long-range interaction yields $\vec{\sigma}_{max}$. Since $\vec{\sigma}_{Kubo}=\vec{\sigma}_{max}$ for a transverse electric field, then, for the purposes of calculating $\vec{\sigma}_{max}$, this modification represents an extension of the Kubo formula from transverse fields to fields of arbitrary polarization. Also, it was noted that finding $\vec{\sigma}_{max}$ actually requires less work than finding $\vec{\sigma}_{Kubo}$ (i.e., it is easier to include screening than to ignore it).

A subsequent publication[14] will present applications of this formalism to concrete physical situations. The purpose of this paper is to present a general discussion of the central issue in a form that leads to results which are applicable to a wide range of diverse systems.

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[1]R. Kubo, J. Phys. Soc. Jpn. **12**, 570 (1957).

[2]This is the same as writing $\nabla\times\mathbf{B}-c^{-1}\partial\mathbf{D}/\partial t=\mathbf{J}_{ext}$, with $\mathbf{D}=\vec{\epsilon}\cdot\mathbf{E}$ and $\vec{\epsilon}=\vec{1}+(i4\pi/\omega)\vec{\sigma}$.

[3]R. Kubo, Rep. Prog. Phys. **29**, 255 (1966).

[4]V. Ambegaokar and W. Kohn, Phys. Rev. **117**, 423 (1960).

[5]For transverse fields, there is no charge density to screen the field, since $\rho=(1/4\pi)\nabla\cdot\mathbf{E}=(i/4\pi)\mathbf{q}\cdot\mathbf{E}=0$.

[6]In Sec. III, H_{SR} was denoted by $\tilde{H}_0$, and H_{LR} was $H_0-\tilde{H}_0$. Examining Eqs. (3.4)–(3.7) shows that the actual definitions are $H_{LR}=-c^{-1}\int d^3x\,\mathbf{J}\cdot(\mathbf{A}_{loc}-\mathbf{A}_{app})$ and $H_{SR}=H_0+c^{-1}\int d^3x\,\mathbf{J}\cdot(\mathbf{A}_{loc}-\mathbf{A}_{app})$.

[7]Any dependence of $\vec{\chi}$ on $\mathbf{E}_{loc}$ would give corrections to (4.21) of higher than first order in $\mathbf{E}_{loc}$.

[8]From $\mathbf{D}=\mathbf{E}+4\pi\mathbf{P}$, we have $\vec{\epsilon}=\vec{1}+4\pi\vec{\chi}$. Combining this with the relation $\vec{\epsilon}=\vec{1}+(i4\pi/\omega)\vec{\sigma}$ from Ref. 2 yields (4.23).

[9]This includes any interaction of an electron with another entity, since such an interaction yields an indirect electron-electron interaction via this entity.

[10]Of course, it is also necessary for the strength of the interaction itself to diverge as $q\to 0$, but this is exactly what it means for the interaction to be long range.

[11]Remember that the division of H_0 into H_{LR} and H_{SR} in Sec. IV was not actually a separation of the long- and short-range interactions, but, rather, a separation of the parts of H_0

which do and do not create a macroscopic electric field $\mathbf{E}_{scr}$ (see Ref. 6). The notation was chosen because only the long-range interactions contribute to H_{LR}.

[12]An improper diagram is one which can be separated into two disconnected pieces by the removal of a single interaction line. A proper diagram is one which is not improper.

[13]T. Izuyama, Prog. Theor. Phys. **25**, 964 (1961).

[14]R. Eykholt and D. L. Mills, Ann. Phys. **171**, 386 (1986).