Kohn's Theorem and Correlation Functions for a Fermi Liquid

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In this paper we derive Kohn's theorem and calculate the spin and current response functions for a Fermi liquid. A magnetic weight is introduced as the limit $\omega/q \to 0$ of the spin response function in analogy to the superfluid weight recently introduced by Scalapino and collaborators. It is conjectured that in this limit both the magnetic-ordered and the Fermi-liquid spin response functions have the same value.

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The correlation-induced metal-insulator (M-I) transition has received considerable attention recently [1,2]. This is driven in part by the broad spectrum of strongly correlated electronic materials that undergo a M-I transition when some parameter, e.g., pressure, temperature, doping, etc., is varied. Some examples of these materials include the vanadium oxides, e.g., V_2O_3 [3], the heavy-fermion (Kondo) insulators, e.g., $Ce_3Bi_4Pt_3$, strontium-doped $La_{2-x}Sr_xTiO_3$ [4], and the high-temperature superconductors, e.g., $La_{2-x}Sr_xCuO_4$ [5]. The correlation-induced M-I transition observed in these materials is usually a phase change that occurs in the absence of an order parameter or an onset of some long range order associated with the transition.

Without an order parameter to characterize the transition between the conducting and insulating phases of a pure material, some other criteria are needed. As argued by Kohn [6] the Drude weight (or charge stiffness), $D_c = \lim_{\omega\to 0} \omega\sigma''(\omega)$, where ω is the frequency and $\sigma''(\omega)$ is the imaginary part of the conductivity, can be used to distinguish between these phases. For an insulator D_c is zero and in the conducting state D_c is nonzero. When the conducting state is a pure metal it is necessary for D_c to be different from zero; however, this is not sufficient to distinguish it from a superconductor. This point has been discussed in great detail by Scalapino, White, and Zhang [7]. One of the important conclusions of these papers [7] is that two distinct limits, as a function of both the momentum transfer $\mathbf{q}$ and ω, of the current-current response function, $\chi_{\mathbf{jj}}(\mathbf{q} = \mathbf{0}, \omega \to 0)$ and $\chi_{\mathbf{jj}}(\mathbf{q} \to \mathbf{0}, \omega = 0)$, the latter related with the optical conductivity, are sufficient to distinguish between the superconducting, metallic, and insulating phases of a pure electronic material.

One of the other key results, which is due to Kohn [6], is the fact that the Drude weight is a ground state property, since it obeys the relation $\partial^2 E(\mathbf{A})/\partial\mathbf{A}^2|_{\mathbf{A}=\mathbf{0}} = \lim_{\omega\to 0}\omega\sigma''(\omega) = D_c$, where $E(\mathbf{A})$ is the energy density in the presence of a vector potential $\mathbf{A}$, such that $\nabla \times \mathbf{A} = \mathbf{0}$ and $\partial\mathbf{A}/\partial t = 0$. This has proven to be a valuable tool, since a number of exact analytic as well as computational techniques are better suited for determining ground state properties [7–9]. However, some care must be taken when computing the second derivative of $E(\mathbf{A})$. As noted by Scalapino, White, and Zhang [7], unless one can follow adiabatically the ground state as the system size is increased, the order of differentiation and the large volume limit give different results for dimensions $d > 1$.

What we show in this Letter is that Kohn's original formulation of the theorem applies to a Fermi liquid, in spite of it being three dimensional ($d = 3$). We compute the second derivative of $E(\mathbf{A})$, which had not yet been evaluated for a Fermi liquid, and relate it to known results for $\sigma(\omega)$. We also calculate the analogous quantities in the spin channel, the spin "Drude" weight (spin stiffness) D_s, and the magnetic weight $D_{\mathcal{M}}$. These are defined in terms of the two limits of the spin-current-current response function $\chi_{\mathbf{j}_s\mathbf{j}_s}(\mathbf{q}, \omega)$ and a relation similar to Kohn's theorem $\partial^2 E(\mathbf{A})/\partial\mathbf{A}^2|_{\mathbf{A}=\mathbf{0}} = D_s$ [8] holds in the spin channel provided we define a convenient spin-dependent vector potential as explained below. We close with some discussion of the various instabilities, superconductivity, spin-density waves (SDW), and the metal-insulator transition.

To demonstrate the validity of Kohn's theorem for a Fermi liquid, we first compute the change in the energy density $\delta E(\mathbf{A})$ to second order in $\mathbf{A}$. The standard expression for δE, first introduced by Landau [10–12], can be written as

$$\delta E = \sum_{\mathbf{p}\sigma} \epsilon^{(0)}_{\mathbf{p}\sigma} \delta n_{\mathbf{p}\sigma} + \frac{1}{2} \sum_{\mathbf{pp}'\sigma\sigma'} f^{\sigma\sigma'}_{\mathbf{pp}'} \delta n_{\mathbf{p}\sigma} \delta n_{\mathbf{p}'\sigma'}, \quad (1)$$

where $\epsilon^{(0)}_{\mathbf{p}\sigma}$ is the quasiparticle energy, $\delta n_{\mathbf{p}\sigma}$ is the change in the momentum distribution function, $f^{\sigma\sigma'}_{\mathbf{pp}'}$ is the quasiparticle interaction, and the volume is set to 1. We consider the change in the energy density in the presence of a spin-dependent vector potential $\mathbf{A}_\sigma$. From this we obtain both the charge and spin stiffnesses. For the charge case we have that $\mathbf{A}_\uparrow = \mathbf{A}_\downarrow = \mathbf{A}$ and for the spin case we have $\mathbf{A}_\uparrow = -\mathbf{A}_\downarrow = \mathbf{A}$, where in both cases

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$\nabla \times \mathbf{A} = \mathbf{0}$ and $\partial \mathbf{A}/\partial t = 0$. This ensures that we have no magnetic $\mathcal{B}$ and electric $\mathcal{E}$ fields present. In principle, if $\mathcal{B} = \mathbf{0}$ and $\mathcal{E} = \mathbf{0}$ then there is no change in E. However, we can imagine that we turn the vector potential on very slowly (adiabatically) such that $\partial \mathbf{A}/\partial t = \mathcal{E}$ for $t < \tau$ and 0 for $t > \tau$, where τ is a time scale that is longer than any relaxation time in the problem. While the vector potential is being adiabatically switched on, there is an electric field that shifts the whole Fermi sphere by an amount $\mathbf{p} \rightarrow \mathbf{p} - \mathbf{A}_\sigma$, where we have set $c = 1$ and $e = 1$. We consider $T = 0$, the temperature limit for which the Landau ansatz becomes exact. The scattering due to the presence of impurities is neglected, since it is a dissipative process and we are interested here only in the reactive part of the conductivity. Expanding $\delta n_{\mathbf{p}\sigma} = n_{\mathbf{p}-\mathbf{A}_\sigma} - n_{\mathbf{p}\sigma}^{(0)}$ to second order in $\mathbf{A}_\sigma$, and substituting in Eq. (1), we find

$$\delta E(\mathbf{A}) = \frac{n}{m^*}\left[\mathbf{A}^2 + \frac{1}{4}\sum_{\sigma\sigma'}\frac{F_1^{\sigma\sigma'}}{3}\mathbf{A}_\sigma \cdot \mathbf{A}_{\sigma'}\right], \quad (2)$$

with n the density of particles of the system, m^* the particle's effective mass, $N(0)$ the density of states at the Fermi surface, and $F_1^{\sigma\sigma'} = N(0) f_1^{\sigma\sigma'}$. The charge and spin stiffnesses follow directly from Eq. (2). For $\mathbf{A}_\uparrow = \mathbf{A}_\downarrow$, we obtain

$$D_c = \frac{n}{m^*}\left(1 + \frac{F_1^s}{3}\right) \quad (3a)$$

and for $\mathbf{A}_\uparrow = -\mathbf{A}_\downarrow$

$$D_s = \frac{n}{m^*}\left(1 + \frac{F_1^a}{3}\right). \quad (3b)$$

To complete Kohn's theorem and to study the limits of the response functions, we need to obtain $\chi_{\mathbf{jj}}(\mathbf{q}, \omega)$ and $\chi_{\mathbf{j}_s\mathbf{j}_s}(\mathbf{q}, \omega)$. In the limit $\mathbf{q} = \mathbf{0}$ this is equivalent to calculating the optical conductivity [11],

$$\omega\sigma''(\omega) = \chi_{\mathbf{jj}}(\mathbf{q} = \mathbf{0}, \omega) + \frac{n}{m}. \quad (4a)$$

For the spin case we can define a spin conductivity $\beta''(\omega)$ as

$$\omega\beta''(\omega) = \chi_{\mathbf{j}_s\mathbf{j}_s}(\mathbf{q} = \mathbf{0}, \omega) + \frac{n}{m}. \quad (4b)$$

In the Fermi-liquid theory $\chi_{\mathbf{jj}}(\mathbf{q}, \omega)$ and $\chi_{\mathbf{j}_s\mathbf{j}_s}(\mathbf{q}, \omega)$ can be calculated directly. We can also obtain them from the appropriate charge response function. To see this consider the spin case where we have

$$\chi_{\rho_s\rho_s}(\mathbf{q}, \omega) = \sum_n \frac{2\omega_{n0} \mid (\rho_{s\mathbf{q}}^\dagger)_{n0} \mid^2}{(\omega + i\delta)^2 - \omega_{n0}^2} \quad (5)$$

and

$$\chi_{\mathbf{j}_s\mathbf{j}_s}(\mathbf{q}, \omega) = \sum_n \frac{2\omega_{n0} \mid (J_{s\mathbf{q}}^\dagger)_{n0} \mid^2}{(\omega + i\delta)^2 - \omega_{n0}^2}, \quad (6)$$

respectively, for the spin-density-density and spin-current-current response functions [13], where $\omega_{n0} = \omega_n - \omega_0$, with ω_0 and ω_n the ground and nth excited state energies. The spin-density-density response, which depends on $\rho_{s\mathbf{q}}^\dagger = \sum_{\mathbf{p}\sigma} \sigma a_{\mathbf{p}+\mathbf{q}\sigma}^\dagger a_{\mathbf{p}\sigma}$, and the spin-current-current response, which is a function of $\mathbf{J}_{s\mathbf{q}}^\dagger = \sum_{\mathbf{p}\sigma}(\mathbf{p}/m)\sigma a_{\mathbf{p}+\mathbf{q}\sigma}^\dagger a_{\mathbf{p}\sigma}$, are related to each other through a continuity equation $\omega_{n0}(\rho_{s\mathbf{q}}^\dagger)_{n0} = \mathbf{q} \cdot (\mathbf{J}_{s\mathbf{q}}^\dagger)_{n0}$, and through the f-sum rule,

$$\frac{n}{m} = \frac{\omega^2}{q^2}\sum_n \frac{2\omega_{n0}}{\omega^2} \mid (\rho_{s\mathbf{q}}^\dagger)_{n0} \mid^2. \quad (7)$$

Combining Eqs. (5), (6), and (7), and using the continuity equation, we obtain

$$\chi_{\mathbf{j}_s\mathbf{j}_s}(\mathbf{q}, \omega) + \frac{n}{m} = \frac{\omega^2}{q^2}\chi_{\rho_s\rho_s}(\mathbf{q}, \omega). \quad (8)$$

A similar expression exists for the density-density $\chi_{\rho\rho}(\mathbf{q}, \omega)$ and current-current $\chi_{\mathbf{jj}}(\mathbf{q}, \omega)$ response functions as well.

To obtain $\chi_{\rho\rho}(\mathbf{q}, \omega)$ and $\chi_{\rho_s\rho_s}(\mathbf{q}, \omega)$, we consider the response of the Fermi liquid to a small external potential that couples to the charge $u_\uparrow = u_\downarrow = u$, and one that couples to the spin $u_\uparrow = -u_\downarrow = u$. The nonequilibrium kinetic equation [10–12]

$$\delta n_{\mathbf{p}\sigma} + \frac{r(\hat{\mathbf{q}} \cdot \mathbf{v}_\mathbf{p})}{[1 - r(\hat{\mathbf{q}} \cdot \mathbf{v}_\mathbf{p})]}\frac{\partial n_\mathbf{p}^{(0)}}{\partial \epsilon_\mathbf{p}^{(0)}}\left(\sum_{\mathbf{p}'\sigma'} f_{\mathbf{pp}'}^{\sigma\sigma'}\delta n_{\mathbf{p}'\sigma'} + u_\sigma\right) = 0, \quad (9)$$

where $r = q/\omega$, provides us with the dynamic change in the distribution function from which we can calculate the linear response $\sum_{\mathbf{p}\sigma}\delta n_{\mathbf{p}\sigma}(\mathbf{q}, \omega) = \chi(\mathbf{q}, \omega)u$. In the limit where $\mathbf{q}$ and ω both tend to zero, the transport properties that follow from nonequilibrium considerations will be connected to ground state properties, as the stiffnesses derived before by considering a static deviation. For $r < 1$ Eq. (9) has a converging Neumann solution which, combined with Eq. (8), leads to

$$\chi_{\mathbf{jj},\mathbf{j}_s\mathbf{j}_s}(\mathbf{q} = \mathbf{0}, \omega \rightarrow 0) = -\frac{n}{m} + \frac{n}{m^*}\left(1 + \frac{F_1^{s,a}}{3}\right). \quad (10)$$

If we now use this result to examine Eqs. (4) in the limit $\omega \rightarrow 0$ and $r \rightarrow 0$, we have

$$\lim_{\omega \rightarrow 0}\omega\sigma''(\omega) = \frac{n}{m^*}\left(1 + \frac{F_1^s}{3}\right) \quad (11a)$$

and

$$\lim_{\omega \rightarrow 0}\omega\beta''(\omega) = \frac{n}{m^*}\left(1 + \frac{F_1^a}{3}\right). \quad (11b)$$

Comparing Eq. (11a) with Eq. (3a) proves Kohn's theorem for a Fermi liquid. The equivalence of Eqs. (11b) and (3b) proves, for a Fermi liquid, the spin analog of Kohn's theorem derived by Shastry and Sutherland [8].

We note that these results are valid for a 3D *infinite system of interacting fermions.* The energy that appears in the relation $\partial^2 E(\mathbf{A})/\partial \mathbf{A}^2|_{\mathbf{A}=\mathbf{0}} = D_{c,s}$, in this case, is the energy calculated for a three-dimensional Fermi liquid where it is implicit that the thermodynamic limit has been taken, i.e., $V \to \infty$. In this sense, these results are quite surprising since when one makes $V \to \infty$ before performing the derivatives, it has been shown that at least in the charge channel one should obtain the superfluid weight $D_{\rm sf}$ [7]. *Therefore, the order in which one calculates the derivatives seems not to be the important point, but rather whether or not one is able to follow the ground state adiabatically.*

The superfluid and magnetic weights are defined in the other limit $\mathbf{q} \to \mathbf{0}$ and $r \to \infty$, respectively, as

$$D_{\rm sf} = \lim_{r\to\infty}\left(\chi_{\mathbf{jj}}(\mathbf{q},\omega) + \frac{n}{m}\right) \tag{12a}$$

and

$$D_{\mathcal{M}} = \lim_{r\to\infty}\left(\chi_{\mathbf{j}_s\mathbf{j}_s}(\mathbf{q},\omega) + \frac{n}{m}\right). \tag{12b}$$

Now for the metallic phase with no superconducting or magnetic long-range order, we have that $D_{\rm sf} = 0$ and $D_{\mathcal{M}} = 0$. This can be seen from the $r \to \infty$ limit of Eq. (9), which does not depend on $\mathbf{q}$ and ω, so that the right side of Eq. (8) vanishes as $1/r^2$.

In the superconducting phase both D_c and $D_{\rm sf}$ are finite. For most of the standard superconductors it was shown that $D_c = D_{\rm sf}$. This follows from some earlier work of Leggett where he showed that the London penetration depth at $T = 0$ for a clean superconductor was given by [13]

$$\lambda_L^{-2}(0) = 4\pi \frac{n}{m^*}\left(1 + \frac{F_1^s}{3}\right). \tag{13}$$

The main point to note is that the superfluid weight $D_{\rm sf}$ is determined by the normal-state Fermi-liquid parameters, since D_c has the same value on both sides of the transition [7]. We also have that for the neutral superfluid, e.g., liquid ^{3}He, the velocity of the Goldstone mode at $T = 0$ is given by

$$c^2 = \frac{D_{\rm sf}}{\chi_c}, \tag{14}$$

and $D_{\rm sf} = D_c$, where $\chi_c = N(0)/(1 + F_0^s) = n^2\kappa$ is the charge susceptibility and κ is the compressibility. From this we get the standard result that the Goldstone mode is just the ordinary hydrodynamic first sound mode with $c^2 = (v_F^2/3)(1 + F_0^s)(1 + F_1^s/3)$ [11,12].

We have spent some time discussing the properties of the superfluid and the connection to normal-state parameters. The reason for this is that we want to make a conjecture, based on an analogy with superfluids, about the spin-density wave (SDW) instability in a metal. The first thing to note is that in the normal state the derivations of D_c and D_s are clearly similar; in the end only F_1^s is replaced by F_1^a in going from the charge to the spin case. If we construct the ratio D_s/χ_s, where $\chi_s = N(0)/(1 + F_0^a)$, we get a velocity given by $c_s^2 = (v_F^2/3)(1 + F_0^a)(1 + F_1^a/3)$. This looks like the spin equivalent of first sound; however, there are no propagating spin waves in the hydrodynamic regime. On the other hand, there are propagating spin-zero sound modes for $T \ll \epsilon_F$. The longitudinal modes propagate only if $F_0^a > 0$, whereas the transverse ones will propagate for any $F_0^a > -1$, i.e., as long as the Fermi liquid is stable. This mode for most values of F_0^a and F_1^a has a quadratic dispersion that depends as well on the applied magnetic field [10,14]. This clearly does not qualify as a normal-state mode whose velocity is given by D_s/χ_s.

There is, however, a regime of the parameter space, recently derived by one of the current authors [15], that has a velocity given by D_s/χ_s. This mode is obtained from the normal-state spin hydrodynamic equations for the case $F_0^a = F_1^a/3$. In this regime the transverse spin wave has a linear dispersion given by $\omega_q = \omega_L \pm c_s q$ [15], where $\omega_L = 2B_z$, with B_z the external magnetic field,

$$c_s^2 = \frac{D_s}{\chi_s}, \tag{15}$$

and

$$\frac{D_s}{\chi_s} = \frac{v_F^2}{3}(1 + F_0^a)^2 .$$

Before we complete the conjecture, we turn now to the SDW instability. While this is known mainly as a short-wavelength phenomenon, the symmetry breaking near the transition creates the periodicity from which the hydrodynamics of long-wavelength spin waves will have the same physical content as their short-wavelength counterpart.

In the following we consider some specific models to make the points, but the conclusions are more general. For the Hubbard model at half filling in the weak coupling limit $U/t \ll 1$, where U is the on-site Coulomb repulsion and t is the hopping matrix element, the mean field ground state is an ordinary commensurate SDW [16]. In the large-U regime this Hamiltonian reduces to the Heisenberg model with $J = 4t^2/U$. At the RPA level $\chi_{\rho_s\rho_s}(\mathbf{q},\omega)$ has been calculated [16] for all values of U/t at half filling. It can be shown that [16,17] $\chi_{\rho_s\rho_s}(\mathbf{q},\omega)$ gives the same result for the two limits, i.e., $\omega \to 0$, $r \to 0$ and $q \to 0$, $r \to \infty$. What this means here is that $D_s = D_{\mathcal{M}}$. For example, in the large-U limit with $J = 4t^2/U$, the RPA gives $D_s = D_{\mathcal{M}} = 2Ja^2$, with a the lattice constant [16,17]. This result is clearly more general than the RPA result. If we examine the spin hydrodynamic equations in the ordered antiferromagnet, it can also be shown that the spin wave velocity is given by [18]

$$c_{\mathcal{M}}^2 = \frac{D_{\mathcal{M}}}{\chi_\perp}, \tag{16}$$

and $D_{\mathcal{M}} = D_s$, where $\chi_\perp$ is the transverse spin susceptibility at $q = 0$.

We have discussed the properties of the charge and spin channels together to emphasize the similarities between them, in particular, for the spin channel when $F_0^a = F_1^a/3$ [15]. There are many qualitative similarities between the superfluid and the SDW phases. At the mean field plus RPA level they are mathematically identical. Our conjecture then is that *D_s has the same value on both sides of the magnetic transition, i.e., the normal-state Fermi-liquid parameters close to the SDW transition temperature T_N determine the magnetic weight $D_{\mathcal{M}}$ in the ordered phase*. This conjecture implies that the normal-state spin-wave mode with $F_0^a = F_1^a/3$ is the one that evolves into the Goldstone mode at the transition. The strong spin fluctuations that are present near an SDW transition could, in fact, force specific relationships between the parameters near T_N. This can be studied experimentally by measuring the spin wave spectrum near the transition. The standard conduction electron spin resonance (CESR) experiments pioneered by Schultz and Dunifer [19] could be used to perform these measurements.

Some brief remarks concerning the nature of the metal-insulator transition are also worth discussing here, although they have been pointed out in other contexts. In particular, we have $D_c \to 0$ as we approach the insulating phase. This could result from $m^*/m \to \infty$ (Brinkman-Rice metal-insulator transition) or $n \to 0$ (Mott metal-insulator transition). It should be noted that $m^*/m \to \infty$ does not necessarily lead to an insulating state. For example, in a Galilean invariant system, $m^*/m = 1 + F_1^s/3$; thus $D_c = n/m$. Clearly m^* could diverge and the system would remain conducting. Another question to be addressed is which electrons contribute to the conductivity. From the derivation we see that only Fermi-surface quantities enter into D_c, i.e., $D_c = \frac{1}{3} N(0) v_F^2 (1 + F_1^s/3)$. This can be put, for a spherical Fermi surface, in the form of Eq. (3a) which suggests that all of the electrons are contributing to D_c. This is no accident of the spherical Fermi surface. What we have is that the vector potential shifts every momentum state by the same amount $\mathbf{p} \to \mathbf{p} - \mathbf{A}$ which corresponds to a shifted, but undistorted Fermi surface. Thus, while it is possible to express D_c in terms of Fermi-surface properties, *all* the electrons contribute to the conducting state. The metal-insulator transition cannot occur with $n \to 0$ unless some other symmetry of the lattice is broken as in an SDW or CDW. If this occurs then exitons could form leading to a critical density below which the material is no longer conducting [2].

To summarize, we have derived Kohn's theorem for a Fermi liquid. In addition, we have proved the equivalent theorem for the spin stiffness in a Fermi liquid. We have also proposed that in the ordered SDW phase $D_{\mathcal{M}} = (1 + F_0^a)n/m^*$, where $F_0^a = F_1^a/3$. We have discussed some of the properties of a Fermi liquid when approaching a metal-insulator transition.

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