Thermal Conductivity in Disordered Interacting-Electron Systems

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We study the heat diffusion and the thermal conductivity of the interacting disordered electron liquid in the metallic regime close to the metal-insulator transition. The heat-diffusion constant provides a direct measurement of the quasiparticle diffusion constant which scales differently from the charge-diffusion coefficient. The thermal conductivity scales like the electrical conductivity establishing the validity of the Wiedemann-Franz law up to the metal-insulator transition.

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The transport coefficients and thermodynamical susceptibilities of interacting disordered electrons close to the metal-insulator transitions have attracted considerable attention recently. Analogies with Fermi liquid have been pointed out,[1] and the scaling parameters of the metal-insulator transition originally introduced by Finkelstein[2] have been related to the spin susceptibility, specific heat, and compressibility of the disordered interacting system.[1,3] The transport coefficients, the corresponding susceptibility, and the associated Fermi-liquid parameters exhibit the remarkable structure

$$\sigma_\rho = D_\rho \left[\frac{dn}{d\mu} \right], \quad D_\rho = \frac{D}{(dn/d\mu)/\rho}, \tag{1}$$

$$\sigma_s = D_s \chi, \quad D_s = \frac{D}{\chi/\chi_0}, \tag{2}$$

with σ_ρ, σ_s, D_s, and D_ρ the charge and spin conductivities and diffusion constants, respectively. $dn/d\mu$ and χ are the charge and spin susceptibilities, and ρ and χ_0 are the corresponding bare noninteracting values.

In a previous Letter[4] we proposed a physical picture of the metal-insulator transition based on the existence of quasiparticles in a disordered system. The quasiparticles are characterized by a density of states z, a singlet and a triplet short-range scattering amplitude $\gamma_s = a^2 \Gamma_s z$ and $\gamma_t = a^2 \Gamma_t z$ where a is the spectral weight of the quasiparticle, and the quasiparticle diffusion constant $D_Q = D/z$. If this picture is correct the specific heat at constant volume should be given by $C_V = \rho z T$, a relation first suggested by Castellani and DiCastro[5] on the basis of a perturbative calculation to lowest order in their disorder and general arguments. Equations (1) and (2) suggest the following expression for the heat-diffusion constant and thermal conductivity:

$$\kappa \equiv \sigma_H = C_V D_H; \quad D_H = D/(C_V/C_V^0) = D_Q, \tag{3}$$

where $C_V^0 = \pi^2/3\rho T$ is the bare noninteracting specific heat. Equation (3) which relates the quasiparticle diffusion constant to an observable quantity, as well as the general structure of Eqs. (1)–(3), follows very naturally if we assume that transport is entirely due to quasiparticles. For this purpose we first discuss a phenomenological transport equation for the quasiparticle distribution $n_\sigma(\epsilon_n, r)$. ϵ_n is a label denoting the energy of a single isolated quasiparticle, and plays the role of $k^2/2m^*$ in the Fermi-liquid theory of clean systems. The energy as a functional of $n_\sigma(\epsilon_n, r)$ is given by

$$E = \sum_\sigma \sum_n \int n_\sigma(\epsilon_n, r) \epsilon_n \, d^d r + \frac{1}{2} \int \sum_{\sigma\sigma'} d^d r \int d^d r' \, \delta N_\sigma(r) f_{\sigma\sigma'} \delta N_{\sigma'}(r'). \tag{4}$$

$f_{\sigma\sigma'}$ is the Landau interaction function which in a strongly disordered system does not depend on angle since at distances larger than the mean free path only s-wave scattering is important. $N_\sigma(r)$ is the total density per spin: $N_\sigma(r) = \sum_n n_\sigma(\epsilon_n, r)$. For long-wavelength disturbances we can write down a kinetic equation for diffusing quasiparticles:

$$0 = \partial n_\sigma/\partial t - D_Q \nabla^2 n_\sigma + (\partial n_\sigma/\partial \epsilon)[-D_Q \nabla^2][\phi_\sigma + \sum_{\sigma'} f_{\sigma\sigma'} \delta N_{\sigma'}]. \tag{5}$$

ϕ_σ is an external potential which is set equal to zero in the discussion of thermal properties. This equation differs in form from a transport equation written down first by McMillan.[6] Its meaning is also very different. The quasiparticle distribution $n_\sigma(\epsilon)$ is a function of the energy of the quasiparticle in isolation and not of the local quasiparticle energy as in McMillan's theory. A detailed derivation of Eq. (5) will be presented in a longer publication.

It is straightforward to show that Eqs. (1)–(3) follow from Eq. (5) with $dn/d\mu$ and D written in terms of the Landau parameters in the standard way. In particular, just as in the clean case the term $\sum_{\sigma'} f_{\sigma\sigma'} \delta N_{\sigma'}$ is of order T^2 for a thermal disturbance

$$\delta n_\sigma = -(\partial n/\partial\epsilon)(\epsilon-\mu)\delta T/T,$$

so that the heat diffusion constant is given by $D_H = D_Q$, without any additional Fermi-liquid corrections.

Relations (3) and (1) are important because they show that the Wiedemann-Franz law ($\kappa/T\sigma_\rho =$const) persists up to the metal-insulator transition in the presence of interactions. This law, which was shown in the early sixties[7] to be valid for noninteracting electrons in a disordered medium, depends only on the Fermi-liquid nature of the ground state and is independent of the scaling of the Fermi-liquid parameters. The identification $D_H = D_Q$ gives us a direct experimental handle on the quasiparticle diffusion constant.

In the following we outline a microscopic derivation of Eq. (3). This derivation validates the more qualitative Fermi-liquid considerations and illustrates a new technique that treats correctly the energy vertex in the presence of disorder. In order to study heat transport we introduce the averaged heat-heat response function

$$\chi_H(r,t) = -i\theta(t)\langle[\tilde{H}(r,t),\tilde{H}(0,0)]\rangle, \tag{6}$$

where $\tilde{H}$ is the grand canonical energy density. Its Fourier transform is expected to have diffusive behavior,

$$\chi_H(q,\omega) = -C_V T D_H q^2/(D_H q^2 - i\omega). \tag{7}$$

The Kubo formula for the thermal conductivity κ,

$$\kappa = -\frac{1}{T}\lim_{\omega\to 0}\lim_{q\to 0}\frac{\omega}{q^2}\,\mathrm{Im}\chi_H(\omega,q)$$

and Eq. (7) lead to the relation $\kappa = C_V D_H$.

The presence of a two-body interaction term in $\tilde{H}$ makes a direct calculation of (6) very difficult. This problem is overcome by expressing $\tilde{H}$ in terms of a more tractable bilinear form. By using the equation of motion for the fermion operator $\psi(\mathbf{r},t)$ in the Heisenberg representation, we can in fact write

$$\tilde{H}(r,t) = \tfrac{1}{2}\sum_\sigma \psi_\sigma^\dagger(r,t)[i\,\partial/\partial t + H_0(r)]\psi_\sigma(r,t),$$

where $H_0(r) = -\nabla^2/2 + v(r) - \mu$ is the single-particle Hamiltonian. Here $v(r)$ is a Gaussian random potential with variance $\langle v(r)v(r')\rangle = \delta(r-r')/2\pi\tau_0 N_0$, and μ is the chemical potential. τ_0 is the scattering time in the Born approximation and N_0 the bare single-particle density of states per spin. In the Matsubara formalism, by introduction of the imaginary time τ, Eq. (6) is then reduced to the following time-ordered product[8]:

$$\chi_H(r-r',t-t') = -\tfrac{1}{2}[-\partial/\partial\tau + H_0(r)]\tfrac{1}{2}[-\partial/\partial\tau' + H_0(r')]\sum_{\sigma\sigma'}\langle T_\tau\psi_\sigma^\dagger(\tilde{r},\tilde{\tau})\psi_\sigma(r,\tau)\psi_{\sigma'}^\dagger(\tilde{r}',\tilde{\tau}')\psi_{\sigma'}(r',\tau')\rangle_{\text{connected}}$$

$$-\delta(r-r')\delta(\tau^+ - \tau')[\langle\tilde{H}(r)\rangle + \tfrac{1}{2}\langle H_{\text{int}}(r)\rangle], \tag{8}$$

where $\tilde{\tau} = \tau^+$, $\tilde{\tau}' = \tau'^+$, $\tilde{r} = r$, $\tilde{r}' = r'$, and H_{int} is the interaction energy per unit volume. The last term in Eq. (8) is derived by commutation of the time derivative in $\tilde{H}$ with the time-ordering operator.

The main difficulty in evaluation of Eq. (8) comes from the terms in which the random potential v explicitly appearing in H_0 outside the T_τ product is averaged (contracted) with some v coming from the time dependence of $\psi,\psi^\dagger$ inside the T_τ product. To overcome this difficulty we consider Eq. (8) for a given impurity configuration. The perturbation theory in interaction is then formally carried out in terms of the noninteracting single-particle Green's functions in the exact eigenstate representation, $G(r,r',i\epsilon_n)$, which is a solution of the equation $[i\epsilon_n - H_0(r)]G(r,r',i\epsilon_n) = \delta(r-r')$. The action of the vertex operator $\tfrac{1}{2}[i\epsilon_n + H_0(r)]$ on the Green's function representing the line leaving the energy density vertex is particularly simple:

$$\tfrac{1}{2}[i\epsilon_n + H_0(r)]G(r,r',i\epsilon_n)$$

$$= i\epsilon_n G(r,r',i\epsilon_n) - \tfrac{1}{2}\delta(r-r'). \tag{9}$$

Thus the usual Feynman rule for the correlation function is modified as follows. At each external vertex, instead of the operator $\tfrac{1}{2}[i\epsilon_n + H_0(r)]$, we introduce two kinds of vertices. The first will be denoted by a circle and is assigned the value $i\epsilon_n$. It represents the first term in Eq. (9). The second is denoted by a dot with a slash on the outgoing Green's function and represents the factor $-\tfrac{1}{2}\delta(r-r')$ in Eq. (9). The rule is to assign a value $-\tfrac{1}{2}$ to this vertex and erase the outgoing Green's function (the line with a slash). Now that the random potential has been eliminated from the external vertex, we per-

$$\chi_H(q,\omega) = \chi_H^{st} + \left\langle\Lambda_H \left| L \right| \Lambda_H\right\rangle + \left\langle\Lambda_H \left| L \right| \Gamma_s \left| L \right| \Lambda_H\right\rangle + \cdots$$

FIG. 1. General structure of χ_H. All renormalizations are absorbed in the static vertex Λ_H, the amplitude Γ_s, and the ladder L. Single-particle Green's functions are not renormalized.
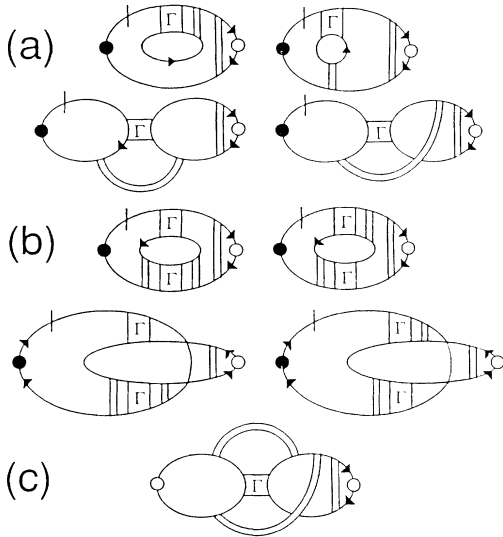
FIG. 2. Diagrams for the dynamic energy-energy correlation function. Double lines represent particle-hole diffusion ladders.

FIG. 3. Diagrams for the dynamic energy-energy correlation function. (d) Ladder and (e) amplitude corrections.

form the usual weak-impurity scattering expansion for the Green's function and the standard impurity averaging techniques are applicable.

We evaluate Eq. (8) for a Coulomb system to lowest order in the disorder strength $t = 1/(2\pi)^2 N_0 D_0$, D_0 being the bare value of the diffusion constant, but to all orders in the scattering amplitudes Γ_s, Γ_t,[9] which characterize the strength of the interactions. We confine our perturbative analysis to the leading corrections close to two dimensions in the spirit of the lowest-order renormalization-group analysis.[2,3] For simplicity, maximally crossed ladder graphs will not be considered.[10] We analyze χ_H in terms of the skeleton graphs[11] drawn in Fig. 1. We separate χ_H into a static part χ_H^{st} which is nonvanishing as $\omega \to 0$ and a dynamic part χ_H^{+-} which is reducible with respect to the ladder L which is the impurity ladder with no interaction connecting the upper and lower lines. We recall[3,12] that L takes the form $L = \zeta^2[-iz\omega + Dq^2 + 1/\tau_{ph}]^{-1}$, where ζ is the wavefunction renormalization, $D = D_0 + \delta D$ is the renormalization diffusion constant, and τ_{ph} is the phase relaxation time. The static part $\chi_H^{st} = C_V T$ where $C_V = C_V^0 + \delta C_V$ and the previous work[5] has identified δC_V with the correction to z so that the identification $C_V = z C_V^0$ can be made to lowest order in t. In order to produce the answers expected by the Landau theory [Eqs. (3) and

(7)], the skeleton expansion must have the form

$$\chi_H = (C_V T) - i\omega C_V^0 T \zeta^2 \Lambda_H^2 / (-i\omega z + Dq^2), \qquad (10)$$

with the additional requirement that $\Lambda_H = z/\zeta$ which can be proved by use of a Ward identity. We have checked that this agrees with the expansion of χ_H to first order in t and all orders in Γ. Before presenting the calculation, we comment on the form of Eq. (10). In the denominator only z appears, instead of a linear combination of z and Γ_s, which would come from summing skeleton diagrams such as the last one in Fig. 1 and all higher-order ones in Γ. A naive reason for this is that an amplitude insertion in the skeleton expansion decouples the energy sum at the vertices, leading to a factor

$$T \sum i\epsilon_n T \sum_{-\omega_n < \epsilon_n < 0} i\epsilon_n T \sum_{-\omega_{m'} < \epsilon_{n'} < 0}$$

which equals $-(16\pi^2)^{-1}\omega^4$ upon analytic continuation and is negligible in the limit $\omega \to 0$. This corresponds to the argument that the Fermi-liquid parameters $f_{pp'}$ do not enter the specific heat and the thermal conductivity since $\sum_{p'} f_{pp'} \delta n_{p'}$ is of order T^2 for δn_p produced by a thermal disturbance. However, while this observation is essentially correct, the detailed diagrammatic expansion in t shows that the amplitude insertion is in fact needed to cancel the mass term τ_{ph}^{-1} which is present in the ladder L, so that in the end, neither the mass term τ_{ph}^{-1} nor Γ appears in the denominator in Eq. (10). The explicit evaluation of χ_H^{+-} to lowest order in t is now presented. Writing $C_V = z C_V^0 = C_V^0 + \delta C_V$, $\zeta = 1 + \delta\zeta$, $D = D_0 + \delta D$, with δC_V, $\delta\zeta$, δD evaluated to lowest order in the disorder, and expanding Eq. (10) to lowest order in the disorder, we find

$$\chi_H^{+-} = -C_V^0 T i\omega / (-i\omega + D_0 q^2) + \delta\chi_H^{+-}(a+b+c) + \delta\chi_H^{+-}(d+e). \qquad (11)$$

$\delta\chi_H^{+-}(a+b+c)$ is the value of Figs. 2(a)–2(c) which contain the corrections to the vertex Λ_H. Explicit calculation shows that it can be expressed in terms of δC_V, and $\delta\zeta$ as follows:

$$\delta\chi_H^{+-}(a+b+c) = -2\delta C_V T i\omega / (-i\omega + D_0 q^2) + i\omega C_V^0 T (2\delta\zeta) / (-i\omega + D_0 q^2). \qquad (12)$$
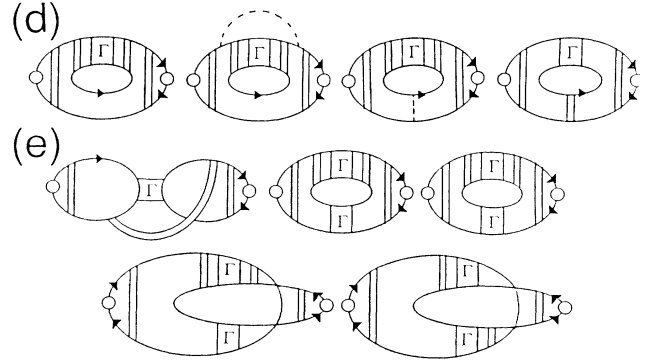
Diagram 2(a) gives the correction to z (i.e., δC_V), whereas diagrams 2(b) and 2(c) give the correction to ζ. $\delta \chi_H^{+-}$(d+e) is the value of Figs. 3(d)–3(e) which contain the corrections to the ladder and the amplitude. We have found that it can be written in the form

$$\delta \chi_H^{+-}(\text{d}+\text{e}) = [i\omega T/(-i\omega + D_0 q^2)^2]C_V^0[-i\omega \delta C_V/C_V^0 + \delta D q^2 - 2\delta\zeta(-i\omega + D_0 q^2)]. \tag{13}$$

By combination of Eqs. (10)–(13), we find that Eqs. (7) and (3) are correct to leading order in t. Thus, in the presence of electron-electron interaction the heat-diffusion constant D_H differs from the charge diffusion constant D_ρ. $D_H/D_\rho \sim 1/z$ and they will scale differently if $z \to 0$ or $z \to \infty$. Nevertheless, the singular corrections to the specific heat introduce additional renormalization to the thermal conductivity. The net result is the validity of the Wiedemann-Franz law up to the metal-insulator transition. In fact, from Eqs. (1) and (3) we find $\kappa = \pi^2/3e^2 T\sigma$ where we used the relations $\sigma = e^2(\partial n/\partial\mu)D_\rho = e^2\rho D$.

These ideas can be checked by the simultaneous measurement of the thermal diffusion constant D_H and the thermal and the electrical conductivities. Since the results presented above rely only on Fermi-liquid considerations, the consistency of the ratio σ/κ would imply the validity of Fermi-liquid theory up to the metal-insulator transition. If in addition we use the results from the ϵ expansion we predict that D_H should remain finite in the presence of spin-orbit scattering while D_ρ vanishes as we approach the metal-insulator transition.

In the presence of magnetic impurities both D_ρ and D_H vanish and so does the ratio D_ρ/D_H. In the strong magnetic field case D_ρ and D_H vanish, but the ratio should remain finite.

Finally, in the case where no spin-orbit or magnetic scattering is present, we expect D_ρ to vanish or to stay finite while D_H should vanish. The ratio D_ρ/D_H should then diverge. We suggest that the analysis of thermal measurements in the light of this present theory could provide a clue to the understanding of the dramatic difference in the critical behavior between compensated and uncompensated semiconductors.

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