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 $C_V=\rho zT$, 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:

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

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

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

$f_{\sigma\sigma'}$ 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:

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

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 ($\kappa/T\sigma_p$=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

$$\tilde H(r,t) = \tfrac12 \sum_\sigma \psi_\sigma^\dagger(r,t)[i\,\partial/\partial t + H_0(r)]\psi_\sigma(r,t),$$

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]:

$$\chi_H(r-r',t-t') = -\tfrac12[-\partial/\partial\tau + H_0(r)]\,\tfrac12[-\partial/\partial\tau' + H_0(r')]\sum_{\sigma\sigma'}\langle T_\tau \psi_\sigma^\dagger(\tilde r,\tilde\tau)\psi_\sigma(r,\tau)\psi_\sigma^\dagger(\tilde r',\tilde\tau')\psi_{\sigma'}(r',\tau')\rangle_{\text{connected}} - \delta(r-r')\delta(\tau^+ - \tau')[\langle\tilde H(r)\rangle + \tfrac12\langle H_{\text{int}}(r)\rangle], \tag{8}$$

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 $\frac12[i\epsilon_n + H_0(r)]$ on the Green's function representing the line leaving the energy density vertex is particularly simple:

$$\tfrac12[i\epsilon_n + H_0(r)]G(r,r',i\epsilon_n) = i\epsilon_n G(r,r',i\epsilon_n) - \tfrac12\delta(r-r'). \tag{9}$$

Thus the usual Feynman rule for the correlation function is modified as follows. At each external vertex, instead of the operator $\frac12[i\epsilon_n + H_0(r)]$, 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 $-\frac12\delta(r-r')$ in Eq. (9). The rule is to assign a value $-\frac12$ 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-

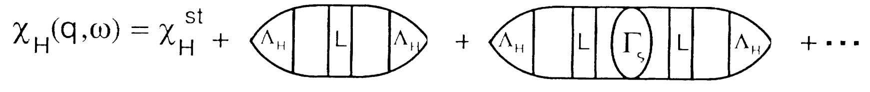

FIG. 1. General structure of χ_H. All renormalizations are absorbed in the static vertex Λ_H, the amplitude Γ_s, and the ladder L. Single-particle Green's functions are not renormalized.

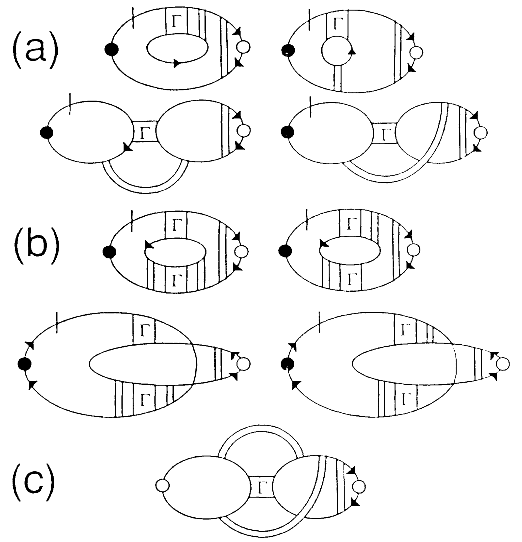

FIG. 2. Diagrams for the dynamic energy-energy correlation function. Double lines represent particle-hole diffusion ladders.

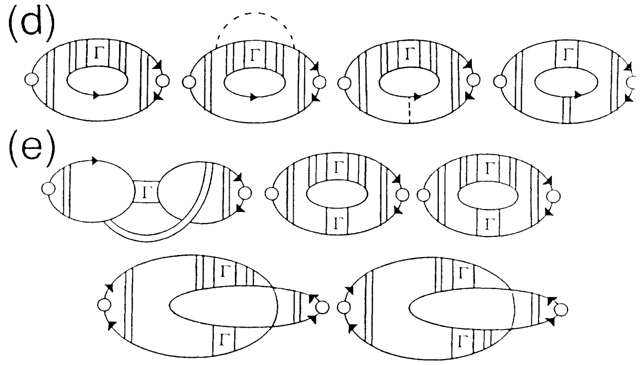

FIG. 3. Diagrams for the dynamic energy-energy correlation function. (d) Ladder and (e) amplitude corrections.

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 $t=1/(2\pi)^2N_0D_0$, 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 $\omega\rightarrow 0$ 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 $L=\zeta^2[-iz\omega+Dq^2+1/\tau_{\text{ph}}]^{-1}$, where ζ is the wave-function renormalization, $D=D_0+\delta D$ is the renormalization diffusion constant, and τ_{ph} is the phase relaxation time. The static part $\chi_H^{\text{st}}=C_VT$ 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 $C_V=zC_V^0$ 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

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

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

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

which equals $-(16\pi^2)^{-1}\omega^4$ upon analytic continuation and is negligible in the limit $\omega\rightarrow 0$. 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 $C_V=zC_V^0=C_V^0+\delta C_V$, $\zeta=1+\delta\zeta$, $D=D_0+\delta D$, 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

$$\chi_H^{+-}=-C_V^0Ti\omega/(-i\omega+D_0q^2)+\delta\chi_H^{+-}(\mathrm{a+b+c})+\delta\chi_H^{+-}(\mathrm{d+e}). \tag{11}$$

$\delta\chi_H^{+-}(\mathrm{a+b+c})$ 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:

$$\delta\chi_H^{+-}(\mathrm{a+b+c})=-2\delta C_VTi\omega/(-i\omega+D_0q^2)+i\omega C_V^0T(2\delta\zeta)/(-i\omega+D_0q^2). \tag{12}$$

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

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

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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