Constrained Quasiparticles and Conduction in Heavy-Fermion Systems

Piers Coleman[a]
Institute for Theoretical Physics, University of California at Santa Barbara, Santa Barbara, California 93106, and Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom
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By extension of the functional-integral treatment of the Kondo-lattice model of heavy-fermion metals to real times, I derive a model transport equation. Frequency- and temperature-dependent conductivities are calculated. Results are contrasted with transport properties of heavy-fermion metals.

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A direct signal of the onset of coherence in heavy-fermion (HF) metals is the sudden reduction in resistivity at low temperatures.[1,2] Most HF metals display a large saturated resistance at high temperature, which drops sharply at low temperature, varying with T^2 near $T=0$. Transport anomalies appear in this low-temperature regime, including a strong sensitivity to disorder, frequency dependence of the conductivity,[3] and sign changes in the magnetoresistance and Hall effect.[2] Qualitatively, these phenomena are understood as a crossover from incoherent single-ion scattering at high temperatures to a low-temperature regime where the strong scattering of conduction electrons off each magnetic ion becomes predominantly elastic, forming a narrow quasiparticle band. Recent de Haas–van Alphen experiments on UPt_3 and $CeCu_6$ [2,4] indicate the development of these narrow f bands. However, despite a measure of success using single-ion models to describe conduction-electron scattering,[5] there is no general framework for describing the coherent low-temperature transport properties in a HF lattice.

In these systems, interactions between the f electrons strongly suppress the low-frequency charge fluctuations, and interaction of the residual f-spin degrees of freedom with the conduction band can be described by a Kondo lattice (KL) model

$$H=\sum_{\mathbf{k},m}E(k)c^\dagger_{\mathbf{k}m}c_{\mathbf{k}m}-(J/N_F)\sum_{\mathbf{R}_j,m,m'}\psi^\dagger_m(j)f_m(j)f^\dagger_{m'}(j)\psi_{m'}(j), \quad (1)$$

where, $\psi^\dagger_m(j)=\sum_k\exp(-i\mathbf{k}\cdot\mathbf{R}_j)c^\dagger_{\mathbf{k}m}$ and $f^\dagger_m(j)$, respectively create a conduction or f electron at site j. For simplicity, spin-orbit coupling is ignored and $N_F=2J+1$ is the electron-spin degeneracy.

In the Kondo model, f-charge fluctuations are suppressed, and so the quasiparticle flux into a given magnetic site i is zero. Schematically, $\sum_m\int\mathbf{j}_m\cdot d\mathbf{S}_i=dn_f/dt=0$, where $\mathbf{j}_m$ is the current of a given spin component. Despite this severe constraint on the currents, f-spin fluctuations given by $\sum_m m\int\mathbf{j}_m\cdot d\mathbf{S}_i=dM_z/dt$ allow a *compensated two-way flow of quasiparticle current* in the different spin channels at site i, allowing quasiparticles of *strong f admixture* to propagate through the lattice. Constrained currents are also implied by path-integral and Gutzwiller treatments of ground-state properties in the Anderson and Kondo lattice.[6–8] In this Letter I show how to construct constrained quasiparticle states and study their response to an external electric field $\mathbf{E}=-\nabla\phi$ coupled to the conduction electrons via the interaction $H_\phi=e\sum_{j,m}\phi(\mathbf{R}_j,t)\psi^\dagger_m(j)\psi_m(j)$.

The space $\{|Q,\alpha\rangle\}$ of KL states with Q f electrons at each magnetic site is constructed by projection from the Fock space $\{|\alpha\rangle\}$ of conduction and f electrons, $P_Q|\alpha\rangle=|Q,\alpha\rangle$. This mapping extends the quasiparticle concept to the KL. Thus, if $a^\dagger_{\mathbf{k}mn}=\alpha_n(k)c^\dagger_{\mathbf{k}m}+\beta_n(k)f^\dagger_{\mathbf{k}m}$ defines an admixed band with a filled Fermi sea $|\phi\rangle=\prod_{k<k_F,m,n}a^\dagger_{\mathbf{k}mn}|0\rangle$, then $|Q\rangle=P_Q|\phi\rangle$ is the constrained Fermi sea, and

$$|Q;\mathbf{k}mn,\ldots,\mathbf{k}'m'n'\rangle=P_Q a^\dagger_{\mathbf{k}mn}\cdots a^\dagger_{\mathbf{k}'m'n'}|\phi\rangle$$

defines the constrained quasiparticles. Using Read and Newns's formalism,[9,10] I recast the constraints as interactions between electrons in the Fock space $\{|\alpha\rangle\}$

$$\langle Q,\beta|e^{-iHt}|Q,\alpha\rangle=\int\mathcal{D}v_j^2(t)\,\mathcal{D}\dot{\theta}_j(t)\langle\beta|Te^{-i\int_0^t H[v,\dot{\theta}]dt'}|\alpha\rangle, \quad (2)$$

where $H[v,\dot{\theta}]=H_{\text{band}}+\sum_j H_f(j)$,

$$H_f(j)=\dot{\theta}_j[n_f(j)-Q]+N_F v_j^2/J+v_j h(j), \quad (3)$$

and $h(j)=\sum_m\{\psi^\dagger_m(j)f_m(j)+\text{H.c.}\}$. The phase velocity variables $\dot{\theta}_j$ play the role of P_Q. Transport properties can now be studied as a $1/N_F$ expansion of this real-time path integral.

Mean-field (MF) behavior in the large-N_F limit is determined by the equations $v_j(t)=-(J/2N_F)\langle\hat{h}(j,t)\rangle_0$, and $\langle n_f(j,t)\rangle_0=Q$, evaluated with use of the MF Hamiltonian $H_0(t)=H[v(t),\dot{\theta}(t)]$. In thermal equilibrium $(v_j,\dot{\theta}_j)=(\tilde{V},E_f)$ and H_0 defines a band of heavy quasiparticles $a_{\mathbf{k}mp}=\cos\delta_{kp}c_{\mathbf{k}m}+\sin\delta_{kp}f_{\mathbf{k}m}$, with energies ϵ_{kp},

($p=\pm$) satisfying $(\epsilon_{kp}-E_f)(\epsilon_{kp}-E_k)-\tilde{V}^2=0$, where $\tan\delta(\epsilon_{kp})=\tilde{V}/(\epsilon_{kp}-E_f)$. The density of states $N^*(\epsilon)=\rho\sec^2\delta(\epsilon)$ is strongly enhanced, where ρ is the conduction electron density of states at the Fermi surface.

I consider dissipation generated by the $O(1/N_F)$ fluctuations about the MF limit, assuming higher-order terms merely renormalize the leading order. To leading order, $H[v,\theta]=H_0+\sum_j H_I(j)$, where

$$H_I(j)=(N_F/J)\delta v_j^2+\delta\dot{\theta}_j n_f(j)+\delta v_j h(j) \tag{4}$$

determines the RPA propagators for the fluctuations, denoted by $[\underline{R}(1,2)]_{\alpha\beta}=\langle r_\alpha(1)r_\beta(2)\rangle$, where $\mathbf{r}(1)=[\delta v(1),\delta\theta(1)]$, and $1\equiv(\mathbf{R},t_1)$. I assume that dissipation is *sufficient to maintain fluctuations in thermal equilibrium,* where they are given by analytic continuation of imaginary time propagators $\underline{R}(\mathbf{q},i\nu_n)$.

I develop the transport theory using real-time electron propagators[11]

$$\underline{G}(1,2)=\begin{bmatrix}\underline{G}^R(1,2) & \underline{G}^K(1,2)\\ \underline{0} & \underline{G}^A(1,2)\end{bmatrix},\qquad \underline{G}^\Lambda=\begin{bmatrix}G^\Lambda & M_{cf}^\Lambda\\ M_{fc}^\Lambda & F^\Lambda\end{bmatrix}, \tag{5}$$

where $\Lambda=R$, A, or K denotes retarded, advanced, and Keldysh propagators. G^Λ, M_{cf}^Λ, and F are the conduction, admixed, and f-electron propagators, respectively. $\underline{G}$ obeys a subtracted Dyson equation $[\underline{G}_0^{-1}-\underline{\Sigma},{}^{\otimes}\underline{G}]_-=0$, where "$\otimes$" denotes convolution over intermediate time and lattice points and $\underline{\Sigma}(1,2)$ is the self-energy.

Because of the retarded nature of the interactions, there is strong frequency dependence of $\underline{\Sigma}(\mathbf{k},\omega,\mathbf{R},T)$, $[(\mathbf{R},T)=\frac{1}{2}(1+2)]$ over the characteristic spin-fluctuation scale $T_K=(E_f^2+\tilde{\Delta}^2)^{1/2}$, where $\tilde{\Delta}=\pi\rho\tilde{V}^2$, so that $\partial\underline{\Sigma}/\partial\omega=O(\underline{\Sigma}/T_K)$. The momentum dependence of $\underline{\Sigma}$ is set by the Fermi wave vector k_F, so that $|\partial\underline{\Sigma}/\partial E_k|=O(\underline{\Sigma}/\mu)\ll|\partial\underline{\Sigma}/\partial\omega|$, and the dependence on E_k can be neglected.[12] Though this does not imply a Migdal theorem for spin fluctuations, it does mean that $\underline{G}$ is a sharp function of E_k. Integrating the Dyson equation with respect to E_k then leads to

$$[\underline{g}_0^{-1}+i\underline{\sigma},{}^{\circ}\underline{g}]_-=0. \tag{6}$$

Here $\underline{g}(\hat{\mathbf{k}})=i\int dE_k\underline{G}(k\hat{\mathbf{k}})/2\pi$, and $\underline{\sigma}(\hat{\mathbf{k}})=\underline{\Sigma}(k_F\hat{\mathbf{k}})$ (with $\mathbf{R}$, t_1, and t_2 suppressed). "$\circ$" denotes time convolution and

$$\underline{g}_0^{-1}=\{\underline{\tau}_c[\mathbf{v}_F\cdot\nabla_R+ie\phi(\mathbf{R},t_1)]+i\underline{H}_0(1)\}\delta(t_1-t_2),\quad \underline{H}_0(1)=\begin{bmatrix}E_k(\mu) & \tilde{V}(1)\\ \tilde{V}(1) & E_f(1)\end{bmatrix},\quad \underline{\tau}_c=\tfrac{1}{2}(1+\sigma_3), \tag{7}$$

where $\mathbf{v}_F=v_F\hat{\mathbf{k}}=\nabla_k E_k$ at the Fermi surface is the conduction-electron group velocity.

As the electric field only couples to the conduction component $g_c^K=\mathrm{Tr}[\underline{\tau}_c\underline{g}^K]$ of the density matrix, on carrying out a gradient expansion of the trace of (7) for slow spatial variation of the electric field I find that transport is determined by the conduction-electron component of the Fermi liquid, expressed in terms of the distribution function $f(\hat{\mathbf{k}},\omega,\mathbf{R},T)=\frac{1}{2}(1-\frac{1}{4}g_c^K)$, where $f=f_0(\omega)=[e^{\beta\omega}+1]^{-1}$ in equilibrium. The current density is given by

$$\mathbf{j}(\mathbf{R},T)=eN_F\rho\int d\kappa f(\hat{\mathbf{k}},\omega,\mathbf{R},T)\mathbf{v}_F, \tag{8}$$

where $d\kappa=d\omega\,d\hat{\mathbf{k}}/4\pi$ and $\kappa\equiv(\omega,k_F\hat{\mathbf{k}})$. f obeys the transport equation

$$[(1-\hat{\partial}_\omega\mathrm{Re}\sigma)\partial_T+(\partial_T\mathrm{Re}\sigma)\hat{\partial}_\omega+\mathbf{v}_F\cdot(\nabla+e\mathbf{E}_0e^{i(\mathbf{q}\cdot\mathbf{R}-\nu_0T)}\hat{\partial}_\omega)]f=I_{fl}[f]+I_i[f]. \tag{9}$$

$\mathrm{Re}\sigma=\tilde{V}\tan\delta(\omega)+\mathrm{Re}\sigma_{fl}$ is a conduction-electron self-energy, where

$$\mathrm{Re}\sigma_{fl}=-\pi\int d\kappa'(\tfrac{1}{2}-f')\boldsymbol{\alpha}\cdot\mathrm{Re}\underline{\mu}(\kappa-\kappa')\cdot\boldsymbol{\alpha} \tag{10}$$

is due to fluctuations, and $\boldsymbol{\alpha}=(t+t',tt')$ $[t=\tan\delta(\omega)]$ couples the electrons to the fluctuations $\underline{\mu}(\mathbf{q},\nu)=(\rho/\pi N_F)\underline{R}(\mathbf{q},\nu-i\delta)$. $\hat{\partial}_\omega$ takes discrete derivatives $\hat{\partial}_\omega f=[f/2\nu_0]_{\omega-\nu_0/2}^{\omega+\nu_0/2}$.

$$I_{fl}[f]=-2\pi\int d\kappa'\boldsymbol{\alpha}\cdot\mathrm{Im}\underline{\mu}(\kappa-\kappa')\cdot\boldsymbol{\alpha}C_{\kappa'}^{\kappa} \tag{11}$$

is the inelastic collision term where $C_{\kappa'}^{\kappa}=A(\kappa,\kappa')+A(\kappa',\kappa)$ describes scattering into and out of the state with $A(\kappa,\kappa')=-\frac{1}{2}\{\hat{f}',1-\hat{f}\}n_0$. Here $n_0=[e^{\beta(\omega-\omega')}-1]^{-1}$, and $\hat{f}=\frac{1}{2}\Sigma_\pm f(\omega\pm\frac{1}{2}i\partial_T)$. Finally,

$$I_i[f]=\frac{n_i}{2\pi^2\rho}\int d\hat{\mathbf{k}}'\sin^2\delta_i(\omega)[f(\hat{\mathbf{k}},\omega,\mathbf{R},T)-f(\hat{\mathbf{k}}',\omega,\mathbf{R},T)] \tag{12}$$

describes elastic impurity scattering with phase shift $\delta_i(\omega)$, impurity density n_i.

Two transport regimes are described by these equations: (1) *Quasiparticle regime* ν_0, $T\ll T_K$. In this regime $\hat{\partial}_\omega\to\partial/\partial\omega$, $\hat{f}(\omega)\to f(\omega)$ and (9) can be rewritten[11] in terms of quasiparticles with energies $\epsilon_{kp}=E_k+\mathrm{Re}\sigma(\epsilon_{kp})$, mass renormalization $Z_{kp}^{-1} = \sec^2\delta(\epsilon_{kp}) + O(1/N_{\rm F})$, and distribution function $n_{\mathbf{k}p} = f(\epsilon_{kp} + e\phi, \hat{\mathbf{k}}, \mathbf{R}, T)$,

$$[\partial_T + Z_{kp}\mathbf{v}_{\rm F}\cdot\nabla_R - \nabla_R(\epsilon_{kp} + e\phi)]n_{\mathbf{k}p} = Z_{kp}I[n_{\mathbf{k}p}]. \tag{13}$$

$Z_{kp}v_f = v_{kp}^* \ll v_{\rm F}$ is the quasiparticle group velocity and $Z_{kp}I$, the renormalized scattering rate. The current of the small conduction component of the Fermi liquid, given in (8), can also be written as a *slow* current of constrained quasiparticles of predominantly f character, $\mathbf{j}(R,T) = eN_{\rm F}\sum_{p,k}\mathbf{v}_{kp}n_{\mathbf{k}p}$. (2) *Finite frequencies* $\nu_0 > T_{\rm K}$. Here, well-defined quasiparticle excitations no longer exist. Making the *Ansatz* $f(\omega,\hat{\mathbf{k}}) = f_0(\omega) - Ae\mathbf{v}_{\rm F}\cdot\mathbf{E}\hat{\partial}_\omega f_0$; then in linear response the equations parallel those of Holstein in the electron-phonon problem,[13] yielding a general expression for the conductivity,

$$\sigma(\mathbf{q},\nu) = \left\langle \frac{ne^2}{m_0} \right\rangle \int_{-\infty}^{\infty} \frac{d\omega}{\nu} \left\langle \frac{f_0(\omega-\nu/2) - f_0(\omega+\nu/2)}{\gamma(\omega,\nu) + i\mathbf{q}\cdot\mathbf{v}_{\rm F} - i\nu} \right\rangle_{\rm FS}, \tag{14}$$

where $\langle ne^2/m_0\rangle = \frac{1}{3}N_{\rm F}\rho e^2 v_{\rm F}^2$, "FS" denotes a Fermi-surface average, and $\gamma = [i\Sigma]_{\omega-\nu/2-i\delta}^{\omega+\nu/2+i\delta}$ describes the scattering rate $\tau_{\rm tr}^{-1} = {\rm Re}\gamma$, and mass renormalization $\lambda(\omega,\nu) = {\rm Im}\gamma/\nu$. $\Sigma_{\rm tr} = \tilde{V}\tan\delta(\omega) + \Sigma_{\rm fl} + \Sigma_i$, where

$${\rm Im}\Sigma_{\rm fl}(\omega - i\delta) = \pi\int d\kappa'\,\boldsymbol{\alpha}\cdot{\rm Im}\underline{\mu}(\kappa-\kappa')\cdot\boldsymbol{\alpha}[1 + n_0(\omega-\omega') - f_0(\omega')][1 - \hat{\mathbf{k}}\cdot\hat{\mathbf{k}}'] \tag{15}$$

is an inelastic-scattering rate, and ${\rm Im}\Sigma_i(\omega - i\delta) = (\pi n_i/\rho)\sin^2\delta_i(\omega)$ is due to impurities. Equation (14) only relies on the scattering rate $\tau_{\rm tr}^{-1}$ being small compared with μ, a weak condition which is still satisfied at high frequencies *beyond the Fermi-liquid regime* studied in earlier work.

To calculate an upper bound on the resistivity, I approximate $\underline{\mu}(\mathbf{q},\nu)$ using the single-impurity, $\mathbf{q}$-independent propagators.[9,10] Actually, q dependence of fluctuations in the lattice is small,[8] reflecting the local nature of the fluctuations, and when combined with the cosine factor in (15), leads to a small reduction in the inelastic-scattering rate, without qualitatively modifying the results.

At low temperatures, the resistivity $\rho(T) = \rho(0) + AT^2$. Here $A = (2/N_{\rm F})^2\rho_U(T/T_c)^2$, and $\rho_U = (h/e^2k_{\rm F})$ is the spin-$\frac{1}{2}$ unitary scattering resistance. $k_{\rm B}T_c = 1/[\pi^2N^*(\mu)]$, where $\frac{1}{3}\pi^2k_{\rm B}^2N_{\rm F}N^*(\mu) = \gamma$, the linear specific heat, so that $A/\gamma^2 = \frac{9}{4}\rho_U[2/(k_{\rm B}N_{\rm F})]^4$. This behavior is a consequence of local spin fluctuations characterized by one energy $T_c \simeq T_{\rm K}$. Figure 1(a) shows that this T^2 regime only persists for a small fraction of $T_{\rm K}$. As $T_{\rm K}$ is approached, oscillator strength in the fluctuations begins to saturate leading to an inflection in the resistance curve, absent in earlier work. Although the semiclassical methods used here are not reliable for $T > T_{\rm K}$ where scattering becomes unitary, by fixing the MF parameters at some $T < T_{\rm K}$, the resistance curves can nevertheless be followed beyond $T_{\rm K}$ giving the rough trend of the resistance which reaches a peak not far above $T_{\rm K}$ as the characteristic fluctuation frequency is exceeded.

At low frequencies $\nu \ll T_{\rm K}$, the conductivity $\sigma(\nu) = \sigma_0/[1 - i\nu\tau_0^*]$ has a Drude peak, with a long quasiparticle lifetime $\tau_0^* = \tau_0(1+\lambda_0)$, as shown by Millis and Lee.[8] Outside this narrow Fermi-liquid regime, strong frequency dependence of the inelastic processes, not contained in previous work, becomes important. Figure 1(b) shows marked reduction in the conductivity for fre-

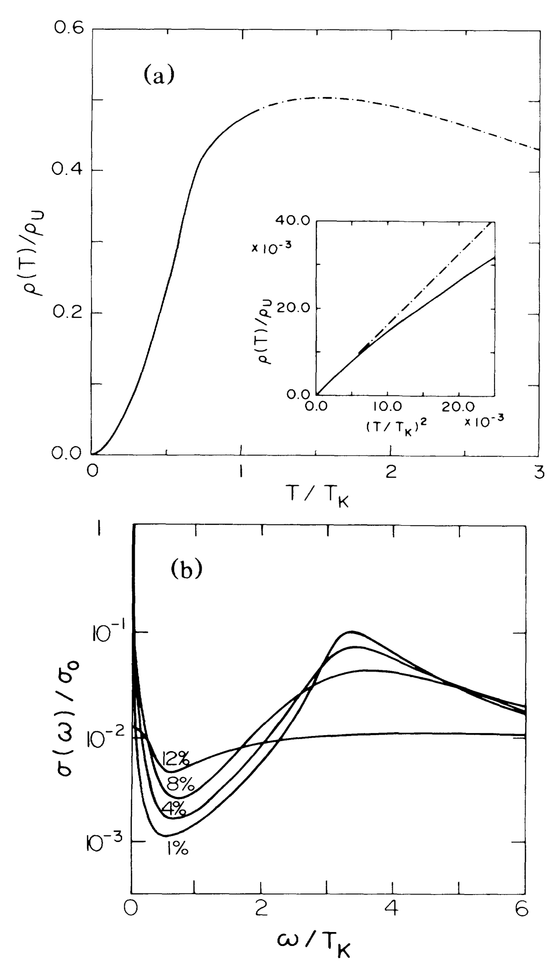

FIG. 1. (a) T dependence of resistivity calculated for $N_{\rm F}=6$, $Q=1$, ignoring impurity scattering; (b) frequency dependence of conductivity calculated for 1%, 4%, 8%, and 12% of unitary scattering impurities, with $N_{\rm F}=6$.

quencies comparable with the hybridization gap around $\nu \simeq E_f$ in this simple model, then an intermediate rise at higher frequencies where interband transitions with smaller inelastic scattering $\gamma(\omega, \nu)$ become important.

In closing, I note that impurity scattering plays an important background role in the transport properties, thermalizing fluctuations, and dissipating the current they carry. In fact, we know that if $k_B T$ becomes less than the quasiparticle scattering rate $1/\tau_0^*$, thermalization is not assured.[14] Though in practice, this is a sufficiently low temperature to be ignored, the presence of impurities is vital to justify the neglect of fluctuation drag and umklapp processes.[13]

With the present simplifications, qualitative features of this model for HF transport are in accord with experiment: The Fermi-liquid scaling of A with γ^2 is correct and by boldly putting $N_F = 2$, $\rho_U = 350$ $\mu\Omega$ cm, $A/\gamma^2 = 1 \times 10^{-5}$ $\mu\Omega$ cm mJ^{-2} mol^2 K^4 is close to the observed value.[15] Secondly, the model has validity beyond this quasiparticle regime, and inflection in the resistance and tendency to saturate at higher frequencies is in accord with the qualitative properties of HF metals.

Detailed application of this model to HF metals requires that splitting of the orbital degeneracy by crystal symmetry and spin-orbit interactions be accounted for. Some of these effects can be included in the MF part of the conduction self-energy, and should have important consequences for the magnetotransport and the high-frequency conductivity. It is hoped that some of these issues can be addressed in the near future.

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(a)Present address: Serin Physics Laboratory, Rutgers University, P.O. Box 849, Piscataway, NJ 08854.

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