Magnetic field induced quantum criticality and the Luttinger sum rule

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We show that when there is a sudden transition from a small to a large Fermi surface at a field induced quantum critical point - similar to what may have been observed in some heavy fermion compounds - an additional term has to be taken into account in the Luttinger-Friedel sum rule. We calculate this additional term for a local model which has a field induced quantum critical point (QCP) and show that it changes abruptly at the transition, such that it satisfies a generalized Luttinger-Friedel sum rule on each side of the transition, and characterizes the two Fermi liquid phases separated by the QCP as a discrete (topological) index.

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I. INTRODUCTION

Quantum critical behavior has been induced in many heavy fermion compounds by reducing the critical temperature of a low temperature phase transition to zero via techniques such as pressure, alloying or an applied magnetic field. The critical behavior of some of these compounds has been understood in the framework of the Wilson renormalization group approach, when the quantum mechanical fluctuations as well as the thermal fluctuations of the order parameter are taken into account. For others, however, where the fluctuations appear to be predominantly local, the extended Wilson approach does not satisfactorily explain the experimental results. There is as yet no fully comprehensive theory of this type of critical behavior so it is a very active area of research, both experimental and theoretical. In heavy fermion compounds, a sudden jump from a small volume to a large volume Fermi surface may have occurred at the field induced transition. As the Luttinger sum rule relates the density of electrons in partially filled bands to the volume of the Fermi surface, this change in volume indicates a sudden change in the degree of localization of the f-electrons. This Fermi surface volume change may also be viewed as supporting the Kondo collapse scenario where the behavior at the quantum critical point has been interpreted as arising from a sudden disappearance of the states at the Fermi level associated with a Kondo resonance or renormalized f-band. To investigate this more fully, we first of all review the steps in the derivation of Luttinger theorem to assess the implications of a system having electrons in partially filled bands and Fermi surfaces with different volumes. We then relate this behavior to that of a local model with a field induced quantum critical point which has a Kondo regime with renormalized f-states at the Fermi level.

We consider a system of non-interacting electrons in eigenstates specified by the set of quantum numbers denoted by α with single particle energies $E_\alpha$. When two-body interaction terms are included the single-particle Green’s function $G_\alpha(\omega)$ can be written in the form,

$$G_\alpha(\omega) = \frac{1}{\omega - \epsilon_\alpha - \Sigma_\alpha(\omega)}, \quad (1)$$

where $\epsilon_\alpha = E_\alpha - \mu$ is the single particle excitation energy relative to the chemical potential $\mu$ and $\Sigma_\alpha(\omega)$ is the proper self-energy term. The expectation value for the total number of electrons in the system, $N$, is then given by

$$N = -\frac{1}{\pi} \sum_\alpha \int_{-\infty}^{0} \lim_{\delta \to 0^+} \left[ \text{Im} G_\alpha(\omega^+) \right] d\omega, \quad (2)$$

where $\omega^+ = \omega + i\delta$ ($\delta > 0$) and we have taken $\mu = 0$. On replacing $G_\alpha(\omega^+)$ in the integrand by $(1 - \Sigma^R_\alpha(\omega^+)) G_\alpha(\omega^+) + \Sigma^I_\alpha(\omega^+ G_\alpha(\omega^+)$, where the prime indicates a derivative with respect to $\omega$, the first integral can be performed to give

$$N = \sum_\alpha \left[ \frac{1}{2} - \frac{1}{\pi} \arctan \left( \frac{\epsilon_\alpha + \Sigma^R_\alpha(0^+)}{\delta + \Sigma^I_\alpha(0^+)} \right) \right]_{\delta \to 0^+} + \sum_\alpha I_\alpha, \quad (3)$$

where

$$I_\alpha = -\frac{1}{\pi} \int_{-\infty}^{0} \text{Im} \left[ \frac{\partial \Sigma_\alpha(\omega^+)}{\partial \omega} G_\alpha(\omega^+) \right]_{\delta \to 0^+} d\omega, \quad (4)$$

and $\Sigma^R_\alpha(\omega^+)$ and $\Sigma^I_\alpha(\omega^+)$ are the real and imaginary parts of $\Sigma_\alpha(\omega)$ respectively.

Note that in deriving the general Eqn. (2) no assumptions of translational invariance or periodicity have been made, so it applies to systems with impurities, including the Friedel sum rule for the single impurity Anderson model if it is expressed in terms of the diagonalized one electron states. It also takes into account any partially filled localized or atomic states.

Luttinger showed, within perturbation theory, that the imaginary part of the self-energy at the Fermi level vanishes, i.e. $[\Sigma_\alpha(0^+)]_{\delta \to 0^+} = 0$ due to phase space restrictions on scattering processes. If this condition holds and $\Sigma^R_\alpha(0)$ is finite, which we denote as condition
(i), then we can simplify Eqn. (3) and rewrite it in the form,

\[ N = \sum_{\alpha} \left[ 1 - \theta (\varepsilon_{\alpha} + \Sigma_{\alpha}^{R}(0)) \right] + \sum_{\alpha} I_{\alpha}. \tag{5} \]

We will refer to this equation as a generalized Luttinger-Friedel sum rule (GLFSR).

Condition (i) is required to be able to define a Fermi surface. If the one-electron states correspond to Bloch states in a lattice with periodic boundary conditions so that the index \( \alpha \) denotes a wave-vector \( k \) and band index \( n \) and a spin index \( \sigma \), then if (i) holds, a Fermi surface can be defined as the locus of points \( k_{F} \) which satisfies

\[ \epsilon_{n,k_{F}} + \Sigma_{n,k_{F}}(0) = 0. \tag{6} \]

In this case Eqn. (5) becomes

\[ N = \sum_{k,\sigma} \left[ 1 - \theta (\varepsilon_{k,\sigma} + \Sigma_{k,\sigma}^{R}(0)) \right] + \sum_{k,\sigma} I_{k,\sigma}. \tag{7} \]

The Luttinger sum rule relating the total number of electrons in partially filled bands to the sum of the volumes of the spin up and spin down Fermi surfaces follows if the Luttinger integral, \( \sum_{k,\sigma} I_{k,\sigma} = 0 \).

If there is a change in the volume of the Fermi surface at a transition, yet no change in the total number of electrons in the states contributing to the sum rule, it follows that the term, \( \sum_{k,\sigma} I_{k,\sigma} \), cannot be zero through the transition. We will exploit the consequences of this observation for a particular model later in this paper.

The relation in Eqn. (5) can be given an interpretation in terms of quasiparticles if \( \Sigma_{\alpha}^{R}(\omega) \) has a finite derivative with respect to \( \omega \) at \( \omega = 0 \) and the derivative, \( \partial \Sigma_{\alpha}^{R}(\omega)/\partial \omega \), is zero evaluated at \( \omega = 0 \), which we denote as condition (ii). The excitation energy of a quasiparticle \( \tilde{\epsilon}_{\alpha} \) can be defined as \( \tilde{\epsilon}_{\alpha} = z_{\alpha} (\epsilon_{\alpha} + \Sigma_{\alpha}^{R}(0)) \), where \( z_{\alpha}(<1) \) is the quasiparticle weight given by

\[ z_{\alpha}^{-1} = \left[ 1 - \frac{\partial \Sigma_{\alpha}^{R}(\omega)}{\partial \omega} \right]_{\omega=0}. \tag{8} \]

If conditions (i) and (ii) are satisfied one can define a total quasiparticle density of states, \( \tilde{\rho}(\omega) \) via

\[ \tilde{\rho}(\omega) = \sum_{\alpha} \delta (\omega - \tilde{\epsilon}_{\alpha}). \tag{9} \]

Note that the quasiparticle density of states is different from the quasiparticle contribution to the spectral density of \( \sum_{\alpha} G_{\alpha}(\omega) \). In terms of the quasiparticles Eqn. (5) takes the form

\[ N = \sum_{\alpha} \left[ 1 - \theta (\tilde{\epsilon}_{\alpha}) \right] + \sum_{\alpha} I_{\alpha}, \tag{10} \]

which sums over the number of occupied free quasiparticle states. Equivalently the first term of the right hand side can be expressed as an integral over the free quasiparticle density of states \( \tilde{\rho}(\omega) \) up to the Fermi level,

\[ N = \int_{-\infty}^{0} \tilde{\rho}(\omega) d\omega + \sum_{\alpha} I_{\alpha}. \tag{11} \]

The existence of long-lived quasiparticle excitations in the neighborhood of the Fermi level is one of the basic assumptions in the phenomenological Fermi liquid theory of Landau, and the microscopic theory provides a criterion for such excitations to exist. For a Fermi liquid a further condition is usually invoked, that the one-electron excitations of the interacting system are adiabatically connected to those of the non-interacting system, which we denote as condition (iii). The proof of the Luttinger sum rule, that \( \sum_{\alpha} I_{\alpha} = 0 \), as given by Luttinger and Ward\textsuperscript{14} requires this third condition (iii) to hold, and adiabatic continuity would appear to be a general requirement in an alternative non-perturbative derivation for a Fermi liquid\textsuperscript{15,16}. However, it is possible for quasiparticle excitations to exist at the Fermi level in a phase in which condition (iii) does not hold, and we have given an example in earlier work\textsuperscript{15,16}. Here we consider a local system which, though not directly applicable as a model of heavy fermion compounds, has a field induced quantum critical point and has a sum rule that mirrors the change in volume of the Fermi surface as may have been observed in some heavy fermion compounds.

\section{Model}

The model we consider is a version of the two impurity Anderson model in the presence of magnetic field. The Hamiltonian for this model takes the form, \( \mathcal{H} = \sum_{i=1,2} \mathcal{H}_{i} + \mathcal{H}_{12} \), where \( \mathcal{H}_{i} \) corresponds to an individual

\begin{figure}[h]
\centering
\includegraphics[width=\columnwidth]{fig1}
\caption{(Color online) A plot of \( h_{c}/J \), where \( h_{c} \) is critical field to induce a transition, as a function of the interaction parameter \( J \) for a particle-hole symmetric model with \( U/\pi \Delta = 5, J_{c} = 2.8272 \times 10^{-5} \) and for an asymmetric model with \( \epsilon_{f}/\pi \Delta = -0.659, U/\pi \Delta = 0.5, J_{c} = 5.4220 \times 10^{-3} \) (dashed line).}
\end{figure}
Anderson impurity model with channel index $i$, 

$$H_i = \sum_{\sigma} \epsilon_{f,i,\sigma} f^\dagger_{i,\sigma} f_{i,\sigma} + \sum_{k,\sigma} \epsilon_{k,i} c^\dagger_{k,i,\sigma} c_{k,i,\sigma} + \sum_{c,k,\sigma} \left( V_{k,i} f^\dagger_{i,\sigma} c_{k,i,\sigma} + h.c. \right) + U_i n_{f,i,\uparrow} n_{f,i,\downarrow},$$

(12)

where $f^\dagger_{i,\sigma}$, $f_{i,\sigma}$, are creation and annihilation operators for an electron at the impurity site in channel $i$ and spin component $\sigma = \uparrow, \downarrow$, and energy level $\epsilon_{f,i,\sigma} = \epsilon_{f,i} - h\sigma$, where $h = g\mu_B H/2$, $H$ is a local magnetic field, $g$ is the g-factor and $\mu_B$ the Bohr magneton. The creation and annihilation operators $c^\dagger_{k,i,\sigma}$, $c_{k,i,\sigma}$ are for partial wave conduction electrons with energy $\epsilon_{k,i}$ in channel $i$, each with a bandwidth $2D$ with $D = 1$. With the assumption of a flat wide conduction band the hybridization factor, $\Delta_i(\omega) = \pi \sum_k |V_{k,i}|^2 \delta(\omega - \epsilon_{k,i})$, can be taken as constant independent of $\omega$. For the inter-impurity interaction Hamiltonian $H_{12}$ we take into account an antiferromagnetic exchange term $J$ and a direct interaction $U_{12}$,

$$H_{12} = 2JS_{f,1} \cdot S_{f,2} + U_{12} \sum_{\sigma,\sigma'} n_{f,1,\sigma} n_{f,2,\sigma'}. \quad (13)$$

The Kondo version of the two impurity model has a long history and was originally put forward to study the competition between the Kondo effect and the intersite RKKY interaction in heavy fermion systems. It was in this context that it was shown to have $T = 0$ phase transition\textsuperscript{17, 22}. Studies based on the two impurity Anderson model in the absence of a magnetic field have revealed a discontinuous change in spectral density at the Fermi level at the transition\textsuperscript{23, 24}. Other studies have shown that the transition is very robust, occurring away from particle-hole symmetry\textsuperscript{22} and even away from the Kondo regime with $U_1 = U_2 = U_{12} = 0$\textsuperscript{15, 19, 20, 27}. The basic picture that emerges is that as the inter-site interaction $J$ is increased from $J = 0$, where the sites are Kondo screened in the case of large $U$, a new universal low energy scale $T^*$ is induced such that on the approach to the transition at $J = J_c$, $T^* \rightarrow 0$. For $J > J_c$, the screening is then predominantly due to the existence of an induced local singlet state, which we will refer to as a localized dimer singlet (LDS) state to distinguish it from the singlet state associated with the Kondo resonance in the regime $J < J_c$. The LDS state can equally well be interpreted as a resonant valence bond (RVB) state.

To demonstrate the field induced transition we consider the model with identical impurities and baths, so we drop the index $i$, in the presence of a local magnetic field $\mu_B H$. We consider a case first of all with particle-hole symmetry and parameters $U/\pi \Delta = 5$ ($\epsilon_f = -U/2$) and $\pi \Delta = 0.01$ (this value will be taken in all calculations) where $J_c$ is $2.8272 \times 10^{-5}$. In the absence of a magnetic field and $J < J_c$, there is a Kondo resonance at the Fermi level with a spectral density $\rho_f(0) = 1/\pi \Delta$. In the LDS phase for $J > J_c$, however, the Kondo resonance disappears leaving a pseudogap with $\rho_f(0) = 0$, reflecting the fact that it costs a finite energy to remove an f-electron and break apart the LDS state (this can be interpreted as the binding energy of the LDS state). This situation can be reversed if we start in the phase with $J > J_c$ and introduce a magnetic field, as an increase in the field leads to a decrease in the energy gain from the LDS formation. At a critical value $h = h_c$, there is an unstable non-Fermi liquid fixed point, such that for $h > h_c$ the system reverts to a phase with the states at the Fermi level associated with the Kondo resonances fully restored, but now polarized by the magnetic field. The greater the value of $J/J_c$, the larger field requirement to induce this transition as can be seen in Fig. 1 where we give a plot of $h_c/J$ as a function of $J/J_c$. As similar transition occurs in the case we consider away from particle-hole symmetry with parameters, $\epsilon_f/\pi \Delta = -0.659, U/\pi \Delta = 0.5, J_c = 5.4220 \times 10^{-3}$, and the critical field $h_c$ for this case is also shown in Fig. 1. The only qualitative difference with the particle-hole symmetric case is that for $J > J_c$, in the absence of a magnetic field, there is some residual f-spectral weight at the Fermi level, as we will show later.

![Image](image.png)

FIG. 2. (Color online) A plot of the quasiparticle weight factors, $z_1 = \Delta_1/\Delta$ and $z_2 = \Delta_2/\Delta$ as a function of the magnetic field $h/h_c$ in the region of the transition for the parameter set $\epsilon_f/\pi \Delta = -0.659, U/\pi \Delta = 0.5, J_c = 5.4220 \times 10^{-3}, J = 5.8482 \times 10^{-3}$, where $h_c/\pi \Delta = 0.20795159$.

### III. RESULTS, DISCUSSIONS AND CONCLUSIONS

To understand this transition in more detail, we calculate the renormalized parameters characterizing the low energy excitations as a function of the magnetic field. We can then see how these parameters vary with $h$ and follow their behavior as we cross the transition. We define a renormalized energy level $\tilde{\epsilon}_{f,\sigma}$, and resonance width $\tilde{\Delta}_{\sigma}$ via

$$\tilde{\epsilon}_{f,\sigma} = z_\sigma \left( \epsilon_{f,\sigma} + \Sigma_\sigma(0) \right), \quad \tilde{\Delta}_\sigma = z_\sigma \Delta_\sigma, \quad (14)$$

where $\Sigma_\sigma(\omega)$ is the self-energy for an individual impurity zero temperature causal Green’s function, $G_{f,\sigma}(\omega)$, given
and $z_{\sigma} = (1 - \partial \Sigma_{\sigma}(\omega)/\partial \omega)_{\omega=0}^{-1}$.

These renormalized parameters can be deduced from NRG excitations in the neighborhood of the low-energy fixed point. The parameter that reflects the loss of quasiparticles as the transition is approached, is the quasiparticle weight factor $z_{\sigma} = \Delta_{\sigma}/\Delta$. This is plotted in Fig. 2 for both spin types as a function of $h/h_c$ for a particle-hole asymmetric model with the parameter set, $\epsilon_f/\pi \Delta = -0.659, U/\pi \Delta = 0.5, J_c = 5.4220 \times 10^{-3}, J = 5.8482 \times 10^{-3}$, where $h_c/\pi \Delta = 0.20795159$, showing that the quasiparticles disappear as the non-Fermi liquid fixed point is approached $h \to h_c$. Though all the quasiparticle parameters tend to zero as $h \to h_c$, their ratios remain finite. The ratio $\hat{\epsilon}_{f,\sigma}/\pi \Delta_{\sigma}$, however, has different limiting values on the two sides of the transition as can be seen in the plot in Fig. 3 for the same parameter set, and corresponds to a phase shift of $\pi/2$. The discontinuity in $\hat{\epsilon}_{f,\sigma}/\pi \Delta_{\sigma}$ arises from a discontinuity in the self-energy term $\Sigma_{\sigma}(0)$ in Eqn. (14). It has also been confirmed from a direct NRG calculation of $\Sigma_{\sigma}(\omega)$. This discontinuity has consequences for the sum rule giving the occupation numbers for the impurity levels.

The generalized Luttinger-Friedel sum rule for each spin component, in terms of renormalized parameters, takes the form,

$$n_{f,\sigma} = \frac{1}{2} - \frac{1}{\pi} \arctan \left( \frac{\hat{\epsilon}_{f,\sigma}}{\Delta_{\sigma}} \right) + I_{f,\sigma},$$

where $n_{f,\sigma}$ is occupation number for the local level with spin $\sigma$ on each impurity. We denote the value of this expression with $I_{f,\sigma} = 0$ by $\tilde{n}_{f,\sigma}$. The value of $n_{f,\sigma}$, can be calculated from a direct NRG calculation or indirectly from an integration over the spectral density $\rho_{f,\sigma}(\omega)$ of the Green’s function $G_{f,\sigma}(\omega)$, and $\tilde{n}_{f,\sigma}$ from the renormalized parameters. Results for $n_{f,\sigma}$, as a function of $h$ is shown in Fig. 4 together with the corresponding results for $\tilde{n}_{f,\sigma}$. For $h > h_c$ there is complete agreement between $n_{f,\sigma}$, and $\tilde{n}_{f,\sigma}$, as expected from the standard Friedel sum rule. For $h < h_c$, we find $I_{f,\sigma} = \frac{1}{2}$ so the shifted value, $\tilde{n}_{f,\sigma} + \frac{1}{2}$, is compared with $\tilde{n}_{f,\sigma}$ in this range. What is clear is that the particle occupation number is continuous through the transition, whereas $\tilde{n}_{f,\sigma}$ is not. Note that in the situation with $\epsilon_f + U/2 > 0$, $I_{f,\sigma}$, has the opposite sign if the arctan is evaluated over the same branch. As $\tilde{n}_{f,\sigma} = n_{f,\sigma} - \frac{1}{2}$ in the range with a LDS, we can interpret $\tilde{n}_{f,\sigma}$ as the contribution from the residual quasiparticles that remain for $h < h_c$. Further evidence backing this interpretation can be seen by look-
As the field value shown in Fig. 5 as a function of $h$, this is just what is expected as a LDS is formed, localizing at the value of the local spectral density at the Fermi level, $\rho_{f,\sigma}(0)$, which is given by

$$\rho_{f,\sigma}(0) = \frac{1}{\pi \Delta} \frac{\Delta^2_{\sigma}}{\epsilon^2_{f,\sigma} + \Delta^2_{\sigma}},$$

in terms of renormalized parameters. The values of $\rho_{f,\sigma}(0)$ for the up and down spins, $\sigma = +(\uparrow), -(\downarrow)$, are shown in Fig. 5 as a function of $h$ through the transition. As the field value $h$ is reduced from above $h_c$ to below $h_c$ there is a sudden loss of spectral weight at the transition. This is just what is expected as a LDS is formed, localizing $1/2$ of an electron of each spin type. As this does not account for all the $f$-electrons, there are still some non-localized quasiparticle states at the Fermi level corresponding to the residual $f$-electrons. This Fermi liquid state ($h < h_c$), which has well defined quasiparticles but does not satisfy the usual sum rule due to the Luttinger integral contribution, corresponds to what in a Kondo lattice model has been described as a fractionalized Fermi liquid. It is also similar to the phenomenological duality model proposed for some heavy fermion systems as well as for the interpretation of the magnetism in some 3d transition metals. The transition as the field $h$ is increased through $h_c$ can therefore be interpreted as a transition from a fractionalized to a normal Fermi liquid. Recently a fermionic and bosonic dimer model for a fractionalized Fermi liquid has been put forward to describe the pseudogap phase of cuprate superconductors and to explain the observed quantum oscillations.

It is interesting to examine the case at particle-hole symmetry where for $J > J_c$ and $h = 0$, there are no quasiparticle states and the local spectral density at the Fermi level is zero. In Fig. 6 the results for $\rho_{f,\sigma}(0)$ for the case with $U/\pi \Delta = 5$, $J = 3.0354436 \times 10^{-5}$ and $J_c = 2.8272 \times 10^{-5}$ showing the sudden increase at the quantum critical point as $h$ increases through $h_c$.

There is a correspondence of these results with what may have occurred in some heavy fermion compounds at the field induced transition: the sudden change in the number of quasiparticle states at the Fermi level and the corresponding increase in the volume of the Fermi surface in line with that expected from the generalized Luttinger-Friedel sum rule. While in the impurity case it is a Fermi liquid for finite $h$ and $T = 0$, it does have finite temperature non-Fermi liquid terms in the vicinity of fixed point at $h = h_c$. There are as yet no exact results for a lattice model of these materials. However, a recent study based on a large-N mean field Hamiltonian does indicate a suppression by the magnetic field of the RKKY coupling relative to the Kondo coupling leading to a transition from a fractionalized Fermi liquid to a heavy Fermi liquid with Kondo correlations. If one can understand what happens to the Luttinger sum rule in passing through a field dependent quantum critical point in the model we have studied, then this can provide a guide to what can happen in more complicated models.

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