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Abstract

The Luttinger Theorem, which relates the electron density to the volume of the Fermi surface in an itinerant electron system, is taken to be one of the essential features of a Fermi liquid. The microscopic derivation of this result depends on the vanishing of a certain integral, the Luttinger integral \( I_L \), which is also the basis of the Friedel sum rule for impurity models, relating the impurity occupation number to the scattering phase shift of the conduction electrons. It is known that non-zero values of \( I_L = \pm \pi/2 \) occur in impurity models classified as singular Fermi liquids. Here we show the same values, \( I_L = \pm \pi/2 \), occur in an impurity model in phases with regular low energy Fermi liquid behavior. Consequently the Luttinger integral can be taken to characterize these phases, and the quantum critical points separating them interpreted as topological.

1. Introduction

The characteristic feature of a Fermi liquid is that its low energy behavior can be understood in terms of interacting quasiparticles and their collective excitations. In the Landau phenomenological formulation [1] of a Fermi liquid it is assumed that the one-electron excitations of these quasiparticles are in 1-1 correspondence with those of the non-interacting system. This correspondence implies that the volume of the Fermi surface of these quasiparticles can be directly related to the electron density, as is the case for the non-interacting system. The microscopic derivation of Fermi liquid theory, clarifying and justifying Landau’s assumptions, was developed in the series of papers by Luttinger and Nozières [2, 3]. The microscopic derivation of the relation between the Fermi surface volume and the electron density given by Luttinger is commonly referred to as the Luttinger theorem or Luttinger sum rule.

Deviations from the Luttinger sum rule, however, have been reported in the results of theoretical calculations for models of strongly correlated electron systems in particular regimes [4–9]. There is also recent experimental evidence [10] that in the underdoped phase of the cuprate superconductors the volume of the Fermi surface corresponds, not to the total electron number \( 1 - p \), but to the doping level \( p \). To investigate the possible origin of such deviations, we first of all take a closer look at the derivation of the Luttinger theorem to see what assumptions are involved in its derivation.

We consider a three dimensional lattice system with Bloch states with energy \( \epsilon_\alpha(k) \), where \( \alpha \) denotes a band index, and a single electron Green’s function \( G_\alpha(k, \omega) \) with a proper self-energy at zero temperature \( \Sigma_\alpha(k, \omega) \) due to interactions,

\[
G_\alpha(k, \omega) = \frac{1}{\omega + \mu - \epsilon_\alpha(k) - \Sigma_\alpha(k, \omega)},
\]

where \( \mu \) is the chemical potential. On the assumption the imaginary part of \( \Sigma_\alpha(k, i\delta) \) vanishes for \( \delta \to 0 \), a Fermi surface with wave-vector \( k_F \) can be defined by

\[
\epsilon_\alpha(k_F) + \Sigma_\alpha(k_F, 0) - \mu = 0.
\]
In order to define quasiparticle excitations we need the further condition that \( \Sigma_\alpha(k, \omega + i\delta) \) behaves asymptotically as \( \Sigma_\alpha(k, \omega + i\delta) \propto \omega^2 \) as \( \omega \to 0 \). This condition was established within perturbation theory by Luttinger [2, 11] as a consequence of the limited phase space for low energy scattering. If we rewrite the self-energy in the form [12, 13],

\[
\Sigma_\alpha(k, \omega) = \mu + \Sigma_\alpha(k, 0) + \omega \Sigma'_\alpha(k, 0) + \Sigma^{\text{rem}}_\alpha(k, \omega),
\]

(3)

where \( \Sigma^{\text{rem}}_\alpha(k, \omega) \) is the remainder term, and we substitute into equation (1), we can rewrite the equation in the form,

\[
G_\alpha(k, \omega) = \frac{z_{\alpha,k}}{\omega - \varepsilon_\alpha(k) - \Sigma_\alpha(k, \omega)},
\]

(4)

where \( z_{\alpha,k} = (1 - \Sigma'_\alpha(k, 0))^{-1} \) and \( \varepsilon_\alpha(k) \), the quasiparticle excitation energy, is given by

\[
\varepsilon_\alpha(k) = z_{\alpha,k} (\mu + \varepsilon_\alpha(k) + \Sigma_\alpha(k, 0)),
\]

(5)

and \( \Sigma_\alpha(k, \omega) = z_{\alpha,k} \Sigma^{\text{rem}}_\alpha(k, \omega) \) is the renormalized self-energy. We can define a free quasiparticle Green’s function, \( \tilde{G}_\alpha^0(k, \omega) \),

\[
\tilde{G}_\alpha^0(k, \omega) = \frac{1}{\omega - \varepsilon_\alpha(k)},
\]

(6)

and a corresponding total free quasiparticle density of states \( \tilde{\rho}_\alpha(\omega) = \sum_{\alpha,k} \delta(\omega - \varepsilon_\alpha(k)) \). The Luttinger theorem is then equivalent to the statement that the total number of electrons corresponds to an integration of the free quasiparticle density of states up to the Fermi level \( \omega = 0 \). The total number of electrons in the system \( N \) can be calculated from the spectral density of the one-electron Green’s function using

\[
N = -\frac{1}{\pi} \sum_{\alpha,k} \int_{-\infty}^{0} \text{Im} G_\alpha(k, \omega + i\delta) d\omega.
\]

(7)

in the limit \( \delta \to +0 \). We can rewrite this expression in the form,

\[
N = -\frac{\text{Im}}{\pi} \sum_{\alpha,k} \int_{-\infty}^{0} \left( 1 - \frac{\partial \Sigma_\alpha(k, \omega + i\delta)}{\partial \omega} \right) G_\alpha(k, \omega + i\delta) d\omega - \frac{\text{Im}}{\pi} \sum_{\alpha,k} \int_{-\infty}^{0} \left( \frac{\partial \Sigma_\alpha(k, \omega + i\delta)}{\partial \omega} \right) G_\alpha(k, \omega + i\delta) d\omega,
\]

(8)

such that the first integral can be explicitly evaluated on using equation (1). The resulting equation for \( N \) is

\[
N = \int_{-\infty}^{0} \tilde{\rho}_\alpha(\omega) d\omega + \frac{I_L}{\pi},
\]

(9)

where \( I_L \) is the Luttinger integral,

\[
I_L = -\text{Im} \int_{-\infty}^{0} \sum_{\alpha,k} \left( G_\alpha(k, \omega) \frac{\partial \Sigma_\alpha(k, \omega)}{\partial \omega} \right) d\omega.
\]

(10)

We will refer to equation (9) as the generalized Luttinger theorem. The standard Luttinger theorem, giving the relation between the electron density and the volume of the Fermi surface, follows from this result with \( I_L = 0 \). The proof given by Luttinger and Ward [14] that \( I_L = 0 \) depends on the validity of the perturbation theory or equivalently that the low energy fixed point of the interacting system is continuously connected to that of the non-interacting system, and hence reduces to the non-interacting fixed point as the interaction terms are adiabatically reduced to zero.

We see that the Luttinger theorem can break down if the self-energy has a singularity at \( \omega = 0 \) such that the steps leading to the definition of a quasiparticle no longer hold. If that is the case then the system is classified as a non-Fermi liquid. Some non-Fermi liquids, however, such as the one dimensional systems known as Luttinger liquids, still satisfy the theorem. Here we investigate another possibility that we can have a Fermi liquid, in that the low energy behaviour of the system can be understood in terms of quasiparticles, but the assumptions leading to the result that \( I_L = 0 \) no longer hold.

Unfortunately there are as yet no really reliable or exact techniques to examine this possibility in lattice models in more than one dimension. However, there are interacting impurity models, where essentially the same question can arise and for which exact and accurate methods have been developed. Probably the most important and well understood interacting impurity model is the Anderson model [15, 16],

\[
\hat{H} = \sum_{\sigma} \epsilon_d d^\dagger d + \sum_{k,\sigma} \epsilon_k c^\dagger_k c_k + \sum_{k,\sigma} (V_k d^\dagger d_c c_{k,\sigma} + \text{h.c.}) + U n_{d,\downarrow} n_{d,\uparrow},
\]

(11)

where \( d^\dagger, d \), are creation and annihilation operators for an electron in a non-degenerate level at the impurity site, with energy \( \epsilon_d \) and spin component \( \sigma = \uparrow, \downarrow \). The parameter \( U(>0) \) is the Coulomb interaction matrix element on the impurity site. The creation and annihilation operators \( c^\dagger_k, c_k \), are for partial wave conduction electrons with energy \( \epsilon_k \) corresponding to a conduction band density of states \( \rho_k(\omega) = 1/2D \) if \( |\omega| < D \),
otherwise $\rho_\ell(\omega) = 0$. The one-electron causal Green’s function at the impurity site $G_d(\omega)$ takes the form,

$$G_d(\omega) = \frac{1}{\omega + i\Delta \text{sgn}(\omega) - \epsilon_d - \Sigma(\omega)},$$  \tag{12}

where $\Delta = \pi \sum_k |V_k|^2 \delta(\epsilon_k)$ and $\Sigma(\omega)$ the local self-energy. The equivalent of the Luttinger sum rule for the impurity is the Friedel sum rule [17], which is essentially a particular application of the more general Luttinger theorem [18]. It gives the occupation of the impurity site $n_d$ in terms of the phase shift of the scattered conduction electrons $\eta$,

$$n_d = \frac{2\eta}{\pi}, \quad \eta = \frac{\pi}{2} - \arctan\left(\frac{\epsilon_d + \Sigma(0)}{\Delta}\right).$$  \tag{13}

The parameters $\tilde{\epsilon}_d$ and $\tilde{\Delta}$ that characterise the free quasiparticles are given by

$$\tilde{\epsilon}_d = z(\epsilon_d + \Sigma(0)), \quad \tilde{\Delta} = z\Delta,$$  \tag{14}

where $z = (1 - \Sigma'(0))^{-1}$. We can define a free quasiparticle density of states for the impurity $\tilde{\rho}_d(\omega)$,

$$\tilde{\rho}_d(\omega) = \frac{1}{\pi} (\omega - \tilde{\epsilon}_d)^2 + \tilde{\Delta}^2,$$  \tag{15}

and the Friedel sum rule given by (13) corresponds to the integration of this quasiparticle density of states up to the Fermi level.

The single impurity Anderson model has a unique low energy fixed point in all parameter regimes corresponding to a Fermi liquid and there is no evidence of any breakdown of the Friedel sum rule. In studies of certain multiple impurity models non-zero values of the Luttinger integral have been reported in certain phases with $J_c = \pm \frac{\pi}{2}$ [19–23]. However, these have been classified as singular Fermi liquids as they have non-analytic low frequency scattering term (for a full discussion of the distinction between regular, singular and non-Fermi liquids see Mehta et al [24]). In the next section we consider the possibility of a finite Luttinger integral term for a two-impurity model with competing phases which, away from particle-hole symmetry, has two distinct regular Fermi liquid low energy fixed points.

2. The model and NRG calculations

The model we consider here describes two quantum dots or impurities coupled by an antiferromagnetic exchange and direct term, with a Hamiltonian $\mathcal{H} = \sum_{\alpha=1,2} \mathcal{H}_\alpha + \mathcal{H}_{12}$, with $\mathcal{H}_\alpha$ corresponding to an individual Anderson impurity model, as given in equation (11) but with an additional index $\alpha = 1, 2$, to label the dots. Each dot is connected to its own conduction bath and hence carry the same $\alpha$ label. The Hamiltonian $\mathcal{H}_{12}$ describes an antiferromagnetic exchange term $J$ and a direct interaction $U_{12}$ between the two dots,

$$\mathcal{H}_{12} = 2J S_{d,1} \cdot S_{d,2} + U_{12} \sum_{\sigma,\sigma'} n_{d,1,\sigma} n_{d,2,\sigma'}.$$  \tag{16}

For simplicity we consider identical dots so we can drop the index $\alpha$ for the impurities.

The model has been well studied, in this form [25, 26], and in earlier forms where the impurities are described by Kondo models [27–32]. The main focus of these studies has been the quantum critical point associated with the development of a locally paired singlet state which occurs at a critical coupling $J = J_c$. For $J < J_c$ any magnetic screening of the impurities is predominantly via the conduction electrons in their respective baths, but for $J > J_c$ the impurities are screened locally by the interaction between them. The Wilson ratios for a spin, charge, staggered spin and charge in the Fermi liquid regimes on both sides of the transition at $J = J_c$ were calculated from the renormalized parameters for the quasiparticles in earlier work [25, 26], and were in complete agreement with exact results found in essentially the same model studied by De Leo and Fabrizio [33]. There is a gap in the local spectral density at the Fermi level in the particle-hole symmetric case $J > J_c$. Here, however, we are concerned with sum rules and spectral densities in the regular Fermi liquid phases away from particle-hole symmetry.

3. Occupation numbers and the Luttinger-Friedel sum rule

We use the numerical renormalization group (NRG) [34, 35] technique to determine the low energy behaviour of this model. If this corresponds to a Fermi liquid fixed point then the low energy effective model takes the same form as the original model but with the parameters $\epsilon_d$, $V_k$, $U$, $J$ and $U_{12}$, replaced by the corresponding renormalized values, $\tilde{\epsilon}_d$, $\tilde{V}_k$, $\tilde{U}$, $\tilde{J}$ and $\tilde{U}_{12}$. There is an additional proviso that all two-body interaction terms have to be normal ordered [12] as the interactions only come into play when two or more quasiparticles are
created from the interacting ground state which plays the role of the vacuum. Though we take \( U_{12} = 0 \) in all cases considered here there are finite values of \( \bar{U}_{12} \) to be taken into account in general. The renormalized parameters (RP) can be deduced from the single particle and two-particle excitations on the approach to the fixed point as has been described elsewhere [36]. We can use the results for \( \bar{r}_d \) and \( \Delta \) and define a quasiparticle impurity occupation number \( \bar{n}_d \) via

\[
\bar{n}_d = \frac{2\eta}{\pi} = 1 - \frac{2}{\pi} \arctan \left( \frac{\bar{r}_d}{\Delta} \right).
\]

We allow for the possibility of a contribution from the Luttinger integral \( I_L \) and so consider the generalized Friedel-Luttinger sum rule for each impurity site which takes the form,

\[
n_d = \bar{n}_d + \frac{2I_L}{\pi},
\]

where \( I_L \) is given by

\[
I_L = -\int_{-\infty}^{0} \text{Im} \, G_d(\omega) \, d\omega \, - \frac{2}{\pi} \left[ \frac{\pi}{2} - \arctan \left( \frac{\epsilon_d + \Sigma_d(0)}{\Delta} \right) \right],
\]

which is derived from the Green’s function given in equation (12), as in the steps following the derivation of equation (10) from equation (8). The total occupation number per impurity site \( n_d \) can be calculated in the NRG from the expectation value of \( \sum_n d_n^\dagger d_n \) in the ground state and \( \bar{n}_d \) from the renormalized parameters deduced from an analysis of the low energy fixed point. Results for both \( n_d \) and \( \bar{n}_d \) are shown and compared in figure 1 as a function of \( J/J_c \) for a parameter set with the impurity level lying above the Fermi level such that for \( J = 0 \), \( n_d < 1 \). For \( J < J_c \) there is a very precise agreement between the values of \( \bar{n}_d \) and \( n_d \). At \( J = J_c \), there is a sudden jump in the value of \( \bar{n}_d \) by 1 which corresponds to a jump in the phase shift \( \eta \) by \( \pi/2 \). This persists for \( J > J_c \) such that the value of \( \bar{n}_d \) exceeds \( n_d \) by 1. The phase shift of \( \pi/2 \) cannot be accounted for by a jump to another branch of the arctan; it suggests that the more general Luttinger-Friedel sum rule given in equation (18) should be used in calculating \( n_d \) from the phase shift.

To check this result we carry out an alternative direct calculation of \( I_L \) by substituting the NRG results for the self-energy and Green’s function in equation (19). The results for \( n_d \) and \( \Sigma_d(0) \) across the transition are shown in figure 2 for the parameter set used in figure 1. They show clearly that the non-zero value of the Luttinger integral \( I_L \) arises from the discontinuity in \( \Sigma_d(0) \) as the value of \( n_d \) as calculated from the integral term on the right hand side of equation (19) is continuous across the transition. The corresponding result for \( I_L \) in figure 3 shows that \( I_L = \pi/2 \) for all values with \( J > J_c \). Also shown are the results for a second parameter set but in this case where the impurity level lies below the Fermi level \( \epsilon_d < 0 \), giving \( I_L = -\pi/2 \) for \( J > J_c \). Note that though we have taken \( U = 0 \) in this case, a finite renormalised \( \bar{U} \) is induced by the exchange term, and is such that \( \bar{U} \to \pi \bar{\Delta} \) as \( J \to J_c \) [25, 26].

To check this behaviour more generally we calculated \( I_L/\pi \) for the parameter set with \( U > \pi \Delta \) and \( J > J_c \) and varied \( \epsilon_d \). The results for \( I_L/\pi \) are shown in figure 4 plotted as a function of \( \epsilon_d \). In all cases, we find a constant value \( I_L/\pi = 1/2 \) over range \( \epsilon_d < -U/2 \) and \( I_L/\pi = -1/2 \) over range \( \epsilon_d > -U/2 \), where the change of sign is at the point with particle-hole symmetry. We conclude that \( I_L \) takes constant values in the different phases.
4. Changes in spectral density across the transition

The jump in the phase shift $\eta$ of $\pi/2$ from the value at $J_-=J_c-\delta$ to that for $J_+=J_c+\delta, \delta \to 0^+$, from equation (17) implies a discontinuity in $\epsilon_d/\Delta$ such that

$$\left[ \frac{\epsilon_d}{\Delta} \right]_{-}^{+} = -1,$$

(20)
or equivalently a discontinuity in the value of $\Sigma(0)$. In the Luttinger-Friedel sum rule this is compensated by the jump in the Luttinger integral to $\pm \pi/2$, so that the value of $n_d$ is continuous through the transition. The sudden discontinuity in $\Sigma(0)$ is however reflected in the spectral density of states $\rho_d(\omega)$ at the impurity site at the Fermi level $\omega = 0$. In terms of the phase shift $\rho_d(0)$ is given by

$$\rho_d(0) = \frac{\sin^2(\eta)}{\pi\Delta} = \frac{1}{\pi\Delta} \frac{\Delta^2}{\tilde{\varepsilon}_d^2 + \Delta^2}. \tag{21}$$

We can calculate this quantity from equation (21) using renormalized parameters as deduced from the low energy fixed point or we can also calculate it from an NRG calculation of the spectral density $\rho_d(\omega)$. In figure 5 we give the results for $\pi \Delta \rho_d(0)$ as a function of $J/J_c$ for the parameter set in figure 1. We see complete agreement between the two sets of results, confirming the Fermi liquid interpretation in the regime $J > J_c$. The mid-point of the discontinuity, indicated by a star in figure 5, corresponds to $\rho_d(0) = 1/2\pi\Delta$, and seems to be a general feature independent of the particular parameter set chosen.

Apart from the sudden jump in the value of $\rho_d(0)$ at $J = J_c$, there is a continuous redistribution of the spectral weight $\rho_d(\omega)$ as $J$ varies through the transition region. In figure 6 we show this change, for the parameter set in figure 1, by comparing the form of $\rho_d(\omega)$ for values of $J/J_c$ slightly below and slightly above the transition. For $J = 0.8J_c$ there is a single broad peak above the Fermi level, which becomes very narrow and shifts to just above the Fermi level at $J = 0.99J_c$. After the transition for $J = 1.01J_c$ there is a sudden drop in the spectral density at the Fermi level and a peak just below the Fermi level. For $J = 1.2J_c$ the peak has shifted to lower energies and broadened with a distinct local minimum in $\rho_d(\omega)$ at the Fermi level. The form of the spectral density in the immediate region of the Fermi level is to a good approximation given by the spectral density due to the free quasiparticles, $\tilde{\rho}_0(\omega)$ given in equation (15), when multiplied by the quasiparticle weight factor $z = \tilde{\Delta}/\Delta$, reflecting the Fermi liquid nature of the low lying excitations. As $J \to J_c$, $\tilde{\varepsilon}_d \to 0$ and $\tilde{\Delta} \to 0$, this quasiparticle expression gives the narrowing of the peak on the approach to the transition. The discontinuity in $\tilde{\varepsilon}_d$ at $J = J_c$ and change of sign from equation (20) gives the shift of the peak across the Fermi level.
We can interpret the loss of spectral weight at the Fermi level as due to formation of the local singlet state, which now requires a finite energy to excite and hence no longer contributes to the elastic scattering of the electrons at the Fermi level. As a consequence, the relation between the zero frequency phase shift of the conduction electrons and the occupation number at the impurity site no longer holds. The Luttinger integral term has to be included in the Friedel sum rule to account for the missing electrons in the local singlet state.

Finally in figure 7 we give the imaginary part of the self-energy \( \text{Im} \Sigma(\omega) \) as a function of \( \omega/T^* \), where \( T^* \) is the renormalized energy scale \( T^* = \pi \Delta / 4 \). For Fermi liquid behavior, as in the single impurity Anderson model, we expect an \( \omega^2 \) form on the scale \( \omega < T^* \). There are some inaccuracies in calculating this quantity from an NRG calculation due to broadening of discrete data, but there is a very reasonable fit to the quadratic form as given in the plot.

5. Conclusions

We have established in this model, away from particle-hole symmetry and for parameter sets with a range of values \( U/\pi \Delta \), that we have three distinct Fermi liquid phases. One of them has the expected value \( I_L = 0 \) for the Luttinger integral. The other two have constant values of \( I_L \) with either \( I_L = \pi/2 \) or \( I_L = -\pi/2 \). As the case with \( I_L = 0 \) includes the case \( J = 0 \) and the single impurity Anderson model, it fits the condition in some definitions of a Fermi liquid that the states of the interacting system correspond to an adiabatic evolution from those of the non-interacting system. This is not the case for the phases with \( I_L = \pm \pi/2 \), where the local singlet electrons do not contribute to the phase shift, but nevertheless they satisfy all the other usual requirements of a Fermi liquid; well defined low energy quasiparticles, with non-singular scattering leading to the usual \( \omega^2 \) terms, and consequent \( T^2 \) low temperature behavior. The case with particle-hole symmetry is different. Though there is a sudden change of phase shift by \( \pi/2 \) at \( J = J_c \), for \( J > J_c \) we find the self-energy has a simple pole, \( \Sigma(\omega) \sim \frac{1}{\omega} \) as \( \omega \to 0 \), and consequently the spectral density goes to zero at the Fermi level.

The different Fermi liquid phases can be classified by the quantum number \( 2I_L/\pi \), which is not associated with any symmetry. This could give a general explanation of puzzling question as to why the transition in this model is so robust, existing not only away from particle-hole symmetry but also for \( U = 0 \). As this quantum number cannot change continuously at any transition between these phases, it implies that the transition at \( J = J_c \) is essentially a topological one. Our results also raise the question as to whether the Luttinger integral can take similar values and modify the standard Luttinger relation in strong correlation lattice models, such as the t-J model [6].

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Figure 7. A plot of \( \text{Im} \Sigma(\omega) \) as a function of \( \omega/T^* \) for the parameter set in figure 1 from the NRG results (stars) with a quadratic fit (circles) for \( J = 2J_c \) and \( T^* = \pi \Delta / 4 = 9.14533 \times 10^{-3} \).
References