Robustness of a local Fermi Liquid against Ferromagnetism and Phase Separation

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We study the properties of Fermi Liquids with the microscopic constraint of a local self-energy. In this case the forward scattering sum-rule imposes strong limitations on the Fermi-Liquid parameters, which rule out any Pomeranchuk instabilities. For both attractive and repulsive interactions, ferromagnetism and phase separation are suppressed. Superconductivity is possible in an s-wave channel only. We also study the approach to the metal-insulator transition, and find a Wilson ratio approaching 2. This ratio and other properties of Sr\textsubscript{1−x}La\textsubscript{x}TiO\textsubscript{3} are all consistent with the local Fermi Liquid scenario.

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For more than a decade now there has been considerable interest in understanding the strong electronic correlations in a variety of materials such as the heavy-fermion metals and related insulators and the perovskites such as the high-T\textsubscript{c} cuprate systems. Recurrent themes in the study of these materials are issues such as unusual Fermi Liquid states characterised by large effective masses, and small Wilson ratios, the proximity to metal-insulator transitions or instabilities towards ferromagnetism, anti-ferromagnetism or superconductivity. Within various frameworks, and to varying degrees of approximation, these systems have been modeled by theories of electrons with local (i.e. momentum-independent) self-energies. For instance, there is much interest in studying correlated systems such as the Hubbard Model using dynamic mean-field theories that become exact in infinite dimension, (based on describing electronic correlations through a local self-energy).

With this background, we investigate the general consequences for Fermi-Liquid Theory, given the microscopic constraint of a local self-energy (arising from quasiparticle correlations alone). We shall show that our local Fermi Liquid (LFL) can never satisfy the Stoner criterion and is robust against instabilities towards ferromagnetism as well as phase separation. This result has strong implications for the use of dynamic mean-field theories to models describing Fermi Liquids. Particularly in the context of recent studies into the criteria necessary for ferromagnetism in metals (due to electronic interactions) as well as problems with phase separation in superconducting models.

In addition, we investigate the approach to the metal-insulator transition (from the metallic side) for our LFL and find a Brinkman-Rice transition with a Wilson ratio, \( R_{\text{BR}} \), near 2 for a wide range of parameters. These results compare very well with measurements of \( R_{\text{BR}} \), the spin susceptibility \( \chi_s \), and the effective mass \( m^*/m \) in the perovskite Sr\textsubscript{1−x}La\textsubscript{x}TiO\textsubscript{3} which becomes insulating as the doping \( x \to 1 \). Furthermore, our LFL scenario makes several predictions which can be measured to test the validity of characterising this system as a LFL. We also investigate the Ward identities and vertex corrections in our theory and contrast our self-consistent LFL with descriptions of Fermi Liquids based on the Gutzwiller approximation which includes some aspects of the local self-energy without being self-consistent. Finally we discuss the limitations of our theory, especially as far as anti-ferromagnetic correlations go. We also briefly outline a natural generalisation of our approach which allows the incorporation of anti-ferromagnetic fluctuations in a self-consistent way.

Our starting point is to take as given that we have a single-band Fermi Liquid with a momentum-independent self-energy \( \Sigma(\omega) \), where \( \text{Im} \Sigma(\omega) \ll \omega \) as \( \omega \to 0 \). Further, we consider the simplest case where the interactions are mediated by the quasiparticles themselves. We emphasise that we do not make the assumption of infinite dimension, although a Fermi Liquid in infinite D would necessarily be a realisation of the LFL theory we present here.

In the spirit of Landau’s microscopic foundation of Fermi-Liquid Theory we determine the structure of the 4-point vertex, given by

\[
\Gamma_{p,p'}(q) = \Gamma_{p,p'}^{\text{IR}}(q) - \int_{p''} \Gamma_{p,p''}(q) G(p''+q) G(p') \Gamma_{p',p''}(q)
\]  

(1)

where \( \Gamma_{p,p'}^{\text{IR}} \) is the irreducible particle-hole vertex, \( G \) is the exact Green’s function and we have dropped the spin indices. Here we introduce the notation \( p = (\mathbf{p}, \omega) \), while \( q = (\mathbf{q}, \Omega) \) denotes the momentum/energy transfer and \( \int_{p''} \) represents the (D+1)-dimensional integral with appropriate measure.

Using the standard analysis, \( \Gamma \) can then be identified with the quasiparticle interaction in the appropriate small momentum transfer limit, with for \( \mathbf{p} \) and \( \mathbf{p}' \) on the Fermi surface and quasiparticle energies \( \omega, \omega' = 0 \),

\[
z^2 f(\mathbf{p}, \mathbf{p}') = \lim_{\Omega \to 0} \lim_{|\mathbf{q}| \to 0} \Gamma_{p,p'}(q).
\]  

(2)

Introducing the Fermi-Liquid parameters and the scattering amplitudes in the standard way, \( f^{(0)} \) then leads to the usual relation

\[
A^{\alpha \alpha}_\ell = \frac{\mathcal{F}^{\alpha \alpha}_\ell}{1 + \mathcal{F}^{\alpha \alpha}_\ell / (2\ell + 1)}
\]  

(3)

where \( N(0) f_{\sigma,\sigma'}(\mathbf{p}, \mathbf{p'}) = \sum_{l} (F_{\ell}^{\sigma} + \delta \sigma' F_{\ell}^{\sigma'}) P_{l} (\mathbf{p} \cdot \mathbf{p'})' \) and \( N(0) \) is the density of states.

Consider the general case of a conserving, \( \Phi \)-derivable theory where the relations between \( \Gamma_{p,p'}^{\text{IR}} \), \( G \) and the self-energy \( \Sigma \) are given by \( \Sigma(p) = \delta \Phi / \delta G(p) \) and \( \Gamma_{p,p'}^{\text{IR}} = \langle i/2 \rangle \delta^2 \Phi / \delta G(p') \delta G(p) \). Integrating the second-order functional derivative then yields

\[
\delta \Sigma(p) = -\langle i/2 \rangle \int_{p''} \Gamma_{p,p'}^{\text{IR}}(0) \delta G(p').
\]  

(4)
In order to understand the constraints imposed by a local self-energy we simply take $\Sigma$ in this equation to be momentum-independent. Together with the symmetry of $\Gamma^{IR}$ under $p \leftrightarrow p'$, this immediately implies that the irreducible vertex is also local, i.e., $\Gamma^{IR}_{p,p'}(0) \rightarrow \Gamma^{IR}_{0,0}(0) = \delta \Sigma(\omega)/\delta G_{loc}(\omega')$ with $G_{loc}(\omega) = \sum_p G(p,\omega)$.

The local irreducible vertex is analytic in $q$ for small $q$ and hence $\Gamma^{IR}_{0,0}(q)$ is also local which in turn implies a local full vertex, $\Gamma_{0,0}(q)$. It then follows from Eq. (2) that $f(p,p')$ is independent of the angles between the momenta, and consequently only s-wave Fermi-Liquid parameters and scattering amplitudes can be non-zero. Moreover, the forward-scattering sum-rule $\sum_e (A^g_e + A^r_e) = 0$ now simplifies to

$$A^g_0 = -A^r_0$$

with $|A^g_0| \leq 1$ and $\Gamma^{IR}$ then implies

$$F^g_0 = -F^r_0/(1+2F^g_0)$$

with $-\frac{1}{2} \leq F^g_0, F^r_0 < \infty$. This relation is plotted in Fig 1 for the repulsive case ($F^g_0 > 0$). For the relatively large $F^g_0$ expected for a strongly correlated local Fermi Liquid, $F^g_0$ very rapidly saturates to $-\frac{1}{2}$. For comparison we also show the results of Müller-Hartmann’s second-order perturbative calculation of the Fermi-Liquid parameters of the Hubbard model in infinite D.

An additional simplification for the local Fermi Liquid is that since $\partial \Sigma/\partial p = 0$, the quasiparticle residue and the effective mass are rather trivially related:

$$z^{-1} = m^*/m.$$  

The microscopic constraint of a local self-energy, is clearly non-trivial. Whereas Fermi-Liquid Theory is characterised in general by an infinite number of Fermi-Liquid parameters, the local Fermi Liquid is quite generally described by only two independent parameters, for instance, $m^*$ and $F^g_0$. The resulting two-parameter phenomenology then implies strong relations between various experimental measurements which can be easily tested to verify the applicability of the LFL scenario. These results are for the case of quasiparticle mediated interactions which lead to Eq. (3). In the case of electron-phonon and single impurity Kondo $\Phi$-derivable Fermi Liquids the interactions are mediated through exchange of phonons or excitations of the impurity-electron singlet which would modify the form of Eq. (3) and hence the relations between the parameters. Finally, we note that the momentum independence of $\Sigma$, also trivially implies that not only the size but also the shape of the Fermi surface are not changed by interactions.

Since we start off with a $\Phi$-derivable theory, our description is conserving by construction and satisfies the Ward identities. The analysis of the 3-point vertices for the charge and spin densities again starts from Eq. (3) and yields that these vertices are local, for small energy/momentum transfers, i.e., $\Lambda^{0}(p) \rightarrow \Lambda^{0}(\omega)$. Setting $\omega = 0$, we consider the $|q|, \Omega \rightarrow 0$ limit: $\Lambda^{r}$ with $r = |q|/\Omega$. Using the Ward identities one then gets:

$$z\Lambda^0 = 1$$

and

$$z\Lambda^\infty = 1/(1 + F^g_0)$$

where $F^g_0$ ($F^r_0$) applies for the charge (spin) density.

The 3-point vertices for the charge and spin currents do retain a trivial momentum dependence, but are otherwise completely unrenormalised (in the interesting two limits). For both spin and charge, in the direction $e\alpha$, we get

$$z\Lambda^0_\alpha = p_\alpha/m^*$$

and

$$z\Lambda^\infty_\alpha = p_\alpha/m^*.$$  

From these relations it can be shown that there are no vertex corrections to the optical conductivity. Without the local assumption, these relations normally do depend on Fermi-Liquid parameters.

We emphasise that all our results hold for arbitrary dimension — provided one has a single-band Fermi Liquid, all that was required was a local self-energy. The dynamical mean-field theories which become exact in infinite dimensions, also have local vertex corrections and unrenormalised current vertices, but our results indicate that (at least in the small $q$ limit) this is a consequence of the local self-energy, rather than infinite $D$, per se.

Now we are in a position to analyse the possible instabilities of our local Fermi Liquid. From Eq. (3) the spin susceptibility $\chi_s = \chi(0)/(1 + F^g_0)$ while the compressibility $\kappa = n^2\chi(0)/(1 + F^g_0)$.

Consider an interaction which is repulsive in the singlet channel, in which case $F^g_0 > 0$ and $-\frac{1}{2} < F^g_0 < 0$. The Stoner criterion, $1 + F^g_0 = 0$, can then never be met and hence the LFL is stable against a ferromagnetic instability. Further, since eqn. (3) cannot generate interactions in higher angular-momentum channels, the LFL is also robust against the Kohn-Luttinger type superconductivity. Also, phase separation is ruled out since $F^g_0 > 0$. The only possible instability is towards anti-ferromagnetism and/or a metal-insulator transition (see below).

For an attractive interaction, one has $-\frac{1}{2} < F^g_0 < 0$ and $F^r_0 > 0$ and there can then be no phase separation since the Pomeranchek instability signaled by the condition $1 + F^g_0 = 0$ can also never be satisfied. (Additionally, ferromagnetism is ruled out since $F^g_0 > 0$.) The only possible instability would be towards the BCS state.

The approach to the metal-insulator transition (from the metallic side) is signaled by a vanishing charge Drude weight $D = ne^2/m^*$. Recall that the Fermi surface volume is unrenormalised by correlations, so the only possible way $D$ can vanish in our framework, is for the effective mass to diverge. The metal-insulator transition is then Brinkman-Rice like. A diverging $m^*$ would imply a diverging density of states, and (although $F^g_0$ is an independent parameter) it is quite natural to expect $F^g_0 \sim N(0)$ to become quite large in this limit. It then follows from Eq. (3) that $F^g_0$ would rapidly approach its limiting value of $-\frac{1}{2}$. This corresponds to the unitarity limit with the scattering amplitude $A^r_0 \rightarrow 1$. Within this scenario, the Wilson ratio $R_w = \chi_s/N(0) = 1/(1 + F^g_0)$ should rapidly saturate at 2. For a strongly correlated system one expects $F^g_0 > 1$ in which case $R_w$ would also be close to 2. In the case of an
attractive interaction, \( F_0^a \) is necessarily positive and then one would find \( R_w < 1 \).

The LFL theory, developed above, seems to apply particularly well to the perovskite system \( \text{Sr}_1-x\text{La}_x\text{TiO}_3 \), which exhibits a metal-insulator transition upon doping. In the \( x = 0 \) limit, \( \text{SrTiO}_3 \) is a band insulator for which band calculations predicts a band mass \( m_b \sim 2m_e \). On the other hand for \( x = 1 \) (corresponding to the \( \frac{1}{2} \)-filled case) \( \text{LaTiO}_3 \) is an insulating anti-ferromagnet. Recent experiments \cite{footnote1} have carefully elucidated the doping dependence in the intermediate metallic regime \( 0.3 < x < 0.95 \), and have shown that this material is very well described by a Fermi Liquid state with a Brinkman-Rice transition as \( x \rightarrow 1 \). Specifically, this is borne out by measurements on the resistivity: \( \rho(T) - \rho_0 \sim AT^2 \) and the specific heat: \( C_V \sim \gamma T \) which show typical Fermi Liquid behaviour for \( 0.3 < x < 0.95 \). Also, the Hall coefficient: \( 1/R_H \sim x \), is electron-like and temperature independent. Upon increasing \( x \), the effective mass diverges and \( \gamma, \chi_\delta \), the inverse Drude weight and the inverse of the square of the plasma frequency, which are all proportional to \( m^* \), increase rapidly. However, even though both \( \gamma \) and \( \chi_\delta \) have a strong doping-dependence, the Wilson ratio \( R_w \propto \chi_\delta / \gamma \) is essentially doping-independent and saturates at a value of \( 2 \). From the low-frequency optical conductivity measurements \cite{footnote1}, the effective mass at \( x = 0.5 \) is about \( m^* \approx 5m_e \) and increases rapidly with increasing \( x \).

The resulting picture of \( \text{Sr}_1-x\text{La}_x\text{TiO}_3 \) is that the electronic response is that of a simple, yet strongly-correlated, single-component Fermi Liquid. This state is strongly correlated in the sense that \( m^* \) and hence \( F_0^a \) are large and that the system exhibits a metal-insulator transition. Yet the Fermi Liquid state is very simple, in that for all doping, it seems to be well described in terms of a single parameter namely, \( m^*(x) \), with the only relevant scale being the Fermi energy \( \epsilon_F \sim k_F^2/2m^*(x) \). (Also, \( F_0^a \) seems to be pinned at \( -\frac{x}{2} \).) This is reminiscent of the simple impurity Kondo problem where strong interaction effects lead to a rather simple low-energy Fermi Liquid state.

All the properties of this material corresponds remarkably well with our local Fermi-Liquid Theory described above. Indeed, if we take a simple parabolic band with \( F_0^a = c_1m^*(x)\sqrt{x} \), using the experimental value of \( \gamma \) to scale the mass in this formula, the resulting theoretical estimation of \( R_w \) agrees quite well with experiment. In Fig. 3 we plot the doping dependence of the Wilson ratio for two plausible choices of \( c_1 \), with the actual experimental results plotted as the triangles. In principle, allowing the coefficient \( c_1 \) to depend on \( x \), would do better, but the main point is that this simple picture captures the essence of the behaviour of \( R_w \). With \( R_w \) close to 2 it is not surprising that superconductivity has not been observed in \( \text{Sr}_1-x\text{La}_x\text{TiO}_3 \). If it were found to be superconducting at very low temperature that would require some small departure from LFL behaviour.

One of the quantities we can estimate is the coefficient of the \( T^2 \) term in the resistivity. The general form for this term has been evaluated \cite{footnote1} to be

\[
\rho(T) = \rho_0 + \left( \frac{3\pi}{10} \frac{\langle |W|^2 \rangle}{m_F a m_n^2 \gamma^2} \right) T^2,
\]

where the coefficient in parentheses is denoted by \( A \). For the local Fermi Liquid the scattering amplitude simplifies to \( \langle |W|^2 \rangle = 8(A_0^2) \) where we have replaced the transport lifetime by the quasiparticle lifetime. This will usually give an order of magnitude estimate for \( A \) and at times it works even better \cite{footnote1}. In general, \( A \) is not strictly proportional to \( \gamma^2 \), however, near the metal-insulator transition our model predicts that \( \langle |W|^2 \rangle \) saturates at a value of 8 and, apart from the small change in \( n \), the dominant change is through \( \gamma^2 \). This is clearly observed in the data for \( \text{Sr}_1-x\text{La}_x\text{TiO}_3 \) with \( x \) close to one. In fact, the simple parabolic band picture gives an estimation of \( A \) which agrees with the experiments up to a factor of two. It should be emphasised that, in principle, \( A \) could be completely dominated by the scattering amplitude — particularly close to an instability. The fact that it is not is a non-trivial vindication of our claim that \( \text{Sr}_1-x\text{La}_x\text{TiO}_3 \) is a local Fermi Liquid.

Another prediction to follow from this theory is the coefficient \( T^3 \ln(T) \) term in the specific heat. This is given by

\[
C_V = \gamma T + \left( \frac{3\pi^2\gamma(A_0^2)}{5F^2} \right) \left( 1 - \frac{\pi^2 A_0^2}{24} \right) T^3 \ln(T/e_\epsilon),
\]

where we have employed the simplifications for a LFL. Near the metal-insulator transition the coefficient in parentheses should saturate to about \( 8\gamma / e_\epsilon \) near the metal-insulator transition. This prediction could be tested by plotting \( C_V / T - \gamma / T^2 \) vs. \( \ln T \) and determining the slope.

A quantity related to the specific heat is the thermopower \( Q = \gamma T / 3n_e \). Since the carriers are electron-like \( \langle e < 0 \rangle \), \( Q \) should be negative. With \( k_B/2e \sim -43\mu V/K \) and \( e_F \sim 4 \times 10^3 \ K \) \( (x = 0.6) \) this gives \( Q \sim -0.04(\mu V/K^2)T \). While getting the numbers right on the thermopower depends on many factors, the trends should be right from our picture. Thus, \( Q/T \) will grow as \( \gamma / n \) as \( x \rightarrow 1 \).

In this model we have shown that \( F_0^{a\alpha} = 0 \) for \( \ell \geq 1 \). While a direct measurement of \( F_0^{a} \) is not possible, a conduction-electron spin-resonance (CESR) experiment could determine the value of \( F_0^{a} \). In such an experiment the spin waves have a dispersion

\[
\omega_q = \omega_L + \left( \frac{1}{3} - \frac{1}{3} \frac{F_0^{a}}{3 + F_0^{a}} \right) q^2 v_F^2 \omega_L,
\]

with \( \omega_L \) the Larmor frequency. In a LFL, the coefficient in parenthesis should reduce to \(-F_0^{a}/3\). Finding such a correspondence between \( \omega_q \) and \( F_0^{a} \) as determined from \( R_w \) would clearly be the most direct evidence for a LFL.

As \( m^* \) increases close to the metal-insulator transition, the only energy scale in the LFL namely, \( e_F \) reduces accordingly. This effect, as well as the building anti-ferromagnetic correlations, should lead to the breakdown of the LFL framework sufficiently close to the transition. For \( \text{Sr}_1-x\text{La}_x\text{TiO}_3 \) the Fermi Liquid state is surprisingly robust and anti-ferromagnetic order sets in only at \( x \sim 0.99 \). What happens beyond \( x = 0.99 \)? Fermi-Liquid Theory, per se, focuses on small momentum-transfer processes and thus does not address the physics of anti-ferromagnetism. In general, keeping track of \((\pi, \pi, \ldots)\)-scattering processes
associated with anti-ferromagnetism is a rather formidable task. However, a generalisation of this approach which allows the incorporation of anti-ferromagnetic fluctuations is to introduce two (bi-partite) sublattices and allow different self-energies on each sublattice while enforcing the constraint of a local self-energy on each sublattice.

It is insightful to compare our results for the LFL with those obtained using the Gutzwiller approximation. This approximation, as used by Brinkman and Rice, discusses the consequences of a local self-energy on each sublattice. The quasiparticle residue $z$ is determined from the theory and the assumption is made that the self-energy is local, i.e., $\delta \Sigma / \delta \Phi = 0$ in order to determine $m^*$. It was shown that the Wilson ratio saturates at 4 when this method is applied to a Galilean invariant system such as liquid $^3$He where $F^s_\alpha \neq 0$. This is clearly in contradiction with the LFL notions we have presented here. The reason is that, with the exception of $D = \infty$, the Gutzwiller approximation is not local as it is assumed to be. Whereas the Gutzwiller approximation is close in spirit to the LFL ideas ($R_w$ does saturate at high pressure and ferromagnetism is suppressed), it is not a proper local Fermi Liquid. In fact, as we have shown, the consequence of a local self-energy for a Galilean invariant system is that $m^*/m = z^{-1} = 1 + F^s_\alpha / 3 = 1$ which is clearly not the case in $^3$He. The Gutzwiller approximation scheme has been recently applied to $\text{Sr}_{1-x}\text{La}_x\text{TiO}_3$ but that calculation again suffers from these subtle inconsistencies regarding locality and would fail to explain the Wilson ratio. A local Fermi Liquid scenario based on the Nozières’ single impurity Kondo Fermi Liquid was introduced by Varma et al. for the heavy-fermion compounds. This is a special case of our LFL theory with $m^*/m = 1 + F_\alpha^s$. This relationship for $m^*$ does not hold in general, but follows from an additional assumption of an unrenormalised compressibility.

In conclusion, we have developed the self-consistent theory of a Fermi Liquid with the microscopic constraint of a local self-energy. We have shown that the local Fermi Liquid is robust against instabilities towards ferromagnetism, phase separation and Kohn-Luttinger superconductivity. The metal-insulator transition in the LFL is Brinkman-Rice-like, and is associated with a Wilson ratio of 2. The properties of our LFL seems to describe the material $\text{Sr}_{1-x}\text{La}_x\text{TiO}_3$ quite well, and we have made several predictions for this material. Our results also have important consequences for dynamic mean-field theories used in infinite D especially when considering states in which all quasiparticles are equivalent – in contrast to anti-ferromagnetic states.

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