Properties of an almost localized Fermi liquid in an applied magnetic field revisited: a statistically consistent Gutzwiller approach

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Abstract
We discuss the Hubbard model in an applied magnetic field and analyze the properties of neutral spin-\(\frac{1}{2}\) fermions within the so-called statistically consistent Gutzwiller approximation. The magnetization curve reproduces in a semiquantitative manner the experimental data for liquid \(^3\)He in the regime of moderate correlations and in the presence of a small number of vacant cells, modeled by a non-half-filled band situation, when a small number of vacancies (\(\sim 5\%\)) is introduced in the virtual fcc lattice. We also present the results for the magnetic susceptibility and the specific heat, in which a metamagnetic-like behavior is also singled out in a non-half-filled band case.

Keywords: correlated fermions, statistically consistent Gutzwiller approach, liquid helium 3, almost-localized Fermi liquid, magnetic properties of Fermi liquid

(Some figures may appear in colour only in the online journal)

1. Introduction

In condensed matter physics, systems with moderate to strong local correlations, such as almost-localized electron systems, heavy-fermion metals, liquid \(^3\)He, and selected cold atomic systems in optical lattices, have been extensively studied during the past decades. On the other hand, starting from the seminal Landau papers on the theory of Fermi liquids [1, 2] as a direct generalization of the concept of an electron gas, it became unquestionable that the interactions between fermions are the source of their non-trivial physical properties even before the Mott transition to the localized state takes place for either sufficiently strong interactions or low density. The original Landau formulation [1], despite being in essence phenomenological, provides a good qualitative rationalization of the observed effective mass enhancement of \(^3\)He atoms in the liquid state [3–6] and that of electrons in metals. However, the Landau Fermi liquid theory turned out to be insufficient to account for specific, more sophisticated effects of the correlations, such as Mott (Mott–Hubbard) localization [7], the appearance of spin-dependent effective masses of quasi-particles [8], or the observation of metamagnetism of itinerant almost-localized and correlated fermions [9]. Note that by correlated fermions or a correlated Fermi liquid we understand a system for which the kinetic or Fermi energy (per particle) is comparable to or even smaller than the interaction energy per particle. Therefore, strictly speaking, one should term those systems strongly interacting; however, that particular phrase is reserved for high-energy interactions of elementary particles. Similar correlated states appear also there, such as, for exam-
A good description of almost-localized systems above the Mott–Hubbard localization [18, 19], as well as leading concomitantly to the so-called upper critical dimensionality (as yet not determined) for fermions. Minimally, it plays the role of a mean-field theory. Among other techniques frequently applied to the Hubbard model are dynamical mean-field theory (DMFT) [21] and the quantum Monte Carlo (QMC) [22] method.

Recently, we have discovered statistical inconsistencies in the GA when one includes the magnetic field via the Zeeman term, and have provided the necessary correction to the GA approach. The extended approach, called the statistically consistent Gutzwiller approximation (SGA), was successfully applied also to the $t-J$ [14, 23, 24], $t-J-U$ [25] and periodic Anderson models [26] to describe both magnetism and superconductivity. The SGA is of the same class approach as the GA (exact in the infinite-dimension limit [7]), but is furthermore consistent from the statistical physics point of view, as explained in detail below (cf. appendix A).

The SGA method we are going to discuss here has its own merits. First, it is analytic and therefore can be applied to infinite-size systems. This means that it can also be compared directly with more numerically oriented approaches, where the lattice size is usually limited. Second, it generalizes the Landau concept of a quasiparticle, as well as providing the corresponding effective single-particle Hamiltonian. Third, it corrects the principal inconsistency of the GA while retaining its attractive qualitative features by providing a testable approach in the vicinity of the border between the moderate and the strong correlation limits. This is the most difficult regime, as here the kinetic and interaction energies are of comparable amplitudes.

In the present paper we have applied the SGA method to the almost-half-filled band situation, where the physics turns out to be non-trivially different from the half-filled case but where the almost-localized character of the system [27–30] is still seen, as discussed below. Such a situation with $N_e < N_L$ (there are fewer fermions than cells) is physically feasible for neutral fermions, whereas for charged fermions (e.g., electrons) a consideration of the non-half-filled band situation requires an additional justification of preserving the charge neutrality of the whole system unless a compensating charge reservoir is assumed. We discuss results concerning magnetization, magnetic susceptibility, and specific heat, as well as the spin-direction dependent effective masses of quasiparticles, in addition to metamagnetism. As an example of its concrete application we have also compared results from our approach for magnetization with the experimentally obtained magnetization curve [31] for liquid $^3$He and found a good semiquantitative agreement. The fitting parameter $U$ places this system in the moderate correlation regime at ambient pressure.

The structure of the paper is as follows. In section 2 we discuss the Hubbard model solution within the statistically consistent Gutzwiller approach (SGA). In section 3 we provide the main results concerning the dependence of the system properties on the applied magnetic field. Section 4 contains conclusions and a brief overview. Appendix A provides some details of the SGA.
A brief methodological remark is in place here. The description is applicable, strictly speaking, to neutral fermions, as we include the applied magnetic field only via the Zeeman term and ignore the Landau-level structure appearing for charged quantum particles. This approach may then be applied to the discussion of both liquid $^3$He and to the neutral cold-atom systems of spin $\frac{1}{2}$ in optical lattice systems.

2. Modeling: statistically consistent Gutzwiller approach (SGA)

Our starting point is the single-band Hubbard Hamiltonian in its translationally invariant form and in an applied magnetic field $H_k$,

$$H = \sum_{\langle ij \rangle, \sigma} t_{ij} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \sigma \hbar \sum i, \sigma \hat{n}_{i\sigma}, \hspace{1cm} (1)$$

where the first term expresses single-particle hopping between sites $i$ and $j$ (with the hopping amplitude $t_{ij} < 0$) and the second describes the intra-atomic repulsive interaction characterized by the Hubbard parameter $U > 0$. The applied magnetic field is introduced via the Zeeman splitting (last term), with $h \equiv \frac{1}{2} g \mu_B H_k$, and for spin $\frac{1}{2}$ we have that $\sigma = \pm 1$. In the case of neutral fermions (atoms in either liquid $^3$He or in an optical lattice) the magnetic field enters the Hamiltonian only via this term. Applying the variational GA procedure [23] we obtain the effective one-particle renormalized Hamiltonian in the form,

$$H_{GA} = \sum_{k, \sigma} (\epsilon_k (d, n, m) - \sigma \hbar) \hat{c}^\dagger_{k\sigma} \hat{c}_{k\sigma} + L U d^2 \hspace{1cm} (2)$$

where $\epsilon_k$ is the single-particle dispersion relation, $L \equiv N_L$ is the number of lattice sites, $d^2$ is the probability of having a doubly occupied site, $n = n_{\uparrow} + n_{\downarrow}$ is the band filling, and $m = n_{\uparrow} - n_{\downarrow}$ is the uniform magnetic polarization per site. The band narrowing factor $q_m(d, m, n)$ is derived from combinatorial calculations in the usual form (a transparent derivation is provided in [9] and [7])

$$q_m = \frac{2}{(n + \sigma m - 2d^2)((1 - n + d^2) + \sqrt{(n - \sigma m - 2d^2)^2})^2} \hspace{1cm} (3)$$

However, in an applied magnetic field the standard self-consistent GA procedure is insufficient. To achieve statistical consistency one needs to introduce additional constraints. The essence of the SGA method is discussed in appendix A. In effect, we introduce a new effective Hamiltonian in the form

$$H_{SGA} \equiv H_{GA} - \lambda_m \left( \sum_{i, \sigma} \sigma \hat{n}_{i, \sigma} - mL \right) - \lambda_n \left( \sum_{i, \sigma} \hat{n}_{i, \sigma} - nL \right), \hspace{1cm} (4)$$

where the Lagrange multipliers $\lambda_m$ and $\lambda_n$ represent the constraints imposed on $m$ and $n$ that their values calculated self-consistently should coincide with those determined variationally. The diagonalization of (4) allows the calculation of the thermodynamic potential functional

$$\mathcal{F}_{SGA} = \frac{1}{\beta} \sum_{k} \ln \left[ 1 + e^{-\beta \epsilon_{k, \sigma}} \right] + L (\lambda_m n + \lambda_m m + U d^2), \hspace{1cm} (5)$$

where the eigenenergies of the quasiparticles are

$$E_{k, \sigma} = \epsilon_k - \sigma (h + \lambda_m) - \mu - \lambda_n. \hspace{1cm} (6)$$

The functional (5) represents the effective Landau functional with order parameters and extra variables expressing the inter-particle correlations.

In order to achieve the condition where the polarization $m$ and the chemical potential $\mu$ determined variationally coincide with those determined in a self-consistent manner, we have effectively introduced corresponding effective fields adding to both $h$ and $\mu$. In essence, this procedure assures the fulfillment of the Bogoliubov theorem, discussed originally in the Hartree–Fock approximation, stating that the introduced effective single-particle approach represents the optimal single-particle representation of the mean-field state. Note also that the Luttinger theorem for the Hamiltonian (4) is obeyed, so that the system is represented by a Fermi liquid, i.e., there is a one-to-one correspondence between the bare states (of energies $\epsilon_k$) and the quasiparticle states ($E_{k, \sigma}$ for $h = 0$). However, a number of renormalizing factors ($q_m, \lambda_m, \lambda_n$) appear; these are determined by the statistical consistency (equilibrium) conditions. The presence of these three parameters, determined either from self-consistency conditions or variationally, represent features which do not appear in the original Landau theory of Fermi liquids. This is the reason why it is termed either as a correlated or an almost-localized Fermi liquid.

The equilibrium values of the parameters and mean field are obtained from the following minimizing procedure of a generalized grand-potential functional (5) with respect to the variables assembled into a vector $\vec{\lambda} \equiv (m, d, n, \lambda_m, \lambda_n)$, representing all relevant quantities, determined from the necessary condition for the minimum

$$\left( \frac{\partial \mathcal{F}}{\partial \lambda_k} \right)_0 = 0, \hspace{1cm} (7)$$

in combination with a comparison of $\mathcal{F}$ values for different possible solutions. Explicitly, the above conditions can be rewritten as a set of five self-consistent equations for the corresponding quantities

$$\lambda_m = -\frac{1}{L} \sum_{k} \frac{\partial}{\partial m_k} f(E_{k, \sigma}) \epsilon_k, \hspace{1cm} (8)$$

$$\lambda_n = -\frac{1}{L} \sum_{k} \frac{\partial}{\partial n_k} f(E_{k, \sigma}) \epsilon_k, \hspace{1cm} (8)$$

$$d = -\frac{1}{L} \sum_{k} \frac{\partial}{\partial d_k} f(E_{k, \sigma}) \epsilon_k, \hspace{1cm} (8)$$

$$n = \frac{1}{L} \sum_{k} f(E_{k, \sigma}), \hspace{1cm} (8)$$

$$m = \frac{1}{L} \sum_{k} \sigma f(E_{k, \sigma}). \hspace{1cm} (8)$$

where $f(E)$ is the Fermi–Dirac distribution function. Note that the first two equations contain the derivatives of the band.
In the case of GA, the fields $\lambda$ narrowing factor with respect to the respective variables and follows next.

The specific heat numerically. A detailed analysis of the results in a non-trivial manner. Therefore we have to determine the variational parameters. Since the potential, we can also determine all relevant thermodynamic determined from (8), reduces to the physical grand potential $\vec{\sigma}$ for the optimal values of the components of vector $\sigma$. The evolution is spin asymmetric, since $q_\sigma$ depends on $m$ in this fashion, with respect to the spin direction $\sigma = \pm 1$.

narrowing factor with respect to the respective variables and would be absent in the ordinary Hartree–Fock approximation. In the case of GA, the fields $\lambda_m = \lambda_n = 0$; this is the limit of weak coupling and represents one of the checks on the method’s reliability. The grand-potential functional evaluated for the optimal values of the components of vector $\lambda$, and determined from (8), reduces to the physical grand potential $\Omega$. Once we have determined the equilibrium thermodynamic potential, we can also determine all relevant thermodynamic quantities. For example, the entropy is

$$S = \frac{d\Omega}{dT} = \left( \frac{\partial F}{\partial T} \right)_0 + \left( \frac{\partial F}{\partial \lambda} \right)_0 \cdot \frac{\partial \lambda}{\partial T},$$

(9)

where subscript ‘0’ labels the equilibrium values of the variational parameters. Since $\left( \frac{\partial F}{\partial \lambda} \right)_0 = 0$ from equation (7), equation (9) simplifies to the form

$$S = -\left( \frac{\partial F}{\partial T} \right)_0 = k_B \sum_{k\sigma} \ln(1 + e^{-\beta E_{k\sigma}}) + \beta E_{k\sigma} f(E_{k\sigma}^0).$$

(10)

The specific heat is then defined in the usual manner by

$$c_V = T \frac{dS}{dT} \bigg|_{n,T,h,V} = -T \frac{\partial^2 F}{\partial T^2} \bigg|_0.$$  

(11)

Note that the variational parameters depend on temperature in a non-trivial manner. Therefore we have to determine the specific heat numerically. A detailed analysis of the results follows next.

3. Results and discussion

3.1. Principal physical properties

To obtain the equilibrium values from solutions of the set of equations (8), we have made use of the scientific library GSL under the GNU license [32]; the precision of the numerical results was $10^{-7}$. In our calculations we set the energy scale in units of the nearest-neighbor hopping $|t|$. We consider a particular closed-packed structure, a three-dimensional face-centered cubic lattice of size $200 \times 200 \times 200$. If not otherwise specified, we have taken into account the second-nearest-neighbor hopping set as $t' = 0.25$, the band filling as $n = 0.97$, and the reduced temperature in the system as $\beta = \frac{1}{k_B T} = 500$, which can be regarded practically as the $T \approx 0$ limit.

Both approaches, the GA as well as the SGA, automatically account for renormalization of the effective mass ($m_\sigma^*$) with respect to the bare band mass ($m_B$) in the form:

$$\frac{m_\sigma^*}{m_B} = q_\sigma^{-1} = \left( \frac{\partial F_k}{\partial E_k} \right)^{-1},$$

(12)

where $q_\sigma$ is the optimized Gutzwiller band narrowing factor defined in (3). In the absence of an applied magnetic field, the effective mass for larger values of the interaction is renormalized appreciably, as detailed in figure 2. However, in an applied magnetic field, in an almost-half-filled band we observe strong asymmetric dependences with respect to the spin direction. This asymmetry with respect to the value of $\sigma = \pm 1$ is caused by the corresponding $m$ dependence of $q_\sigma$.

The curves terminate at the saturation point $m = n$, where simultaneously $m_\uparrow = m_B$ and the spin-minority quasiparticle subband becomes empty. Parenthetically, the saturation point may thus be used to determine the value of the bare band mass, $m_B$, as the Hubbard interaction is then switched off. This spin-dependent mass renormalization of quasiparticles in the strong correlation regime has been discussed extensively in the literature [30, 33–35], and observed experimentally by means of de Haas–van Alphen oscillations in strong magnetic fields [36, 37]. It thus represents a crucial new concept, which does not appear in the standard Landau Fermi liquid (LFL) theory.

In figure 3 we show a family of magnetization curves as a function of the reduced magnetic field ($h \equiv \mu_B H_B$). In comparison to the results obtained within the GA [9, 38] we do not observe any spectacular metamagnetic transition for $n < 1$. The magnetization curves, especially in the intermediate interaction regime, are rather smooth and saturate gradually. Nonetheless we observe a weak kink, which we qualify as metamagnetic-like behavior. Indeed, this kink can be singled out clearly on the field dependence of the magnetic susceptibility and the specific heat curves, as shown in figures 4 and 5, respectively.

One can say that the presence of both spin-dependent masses and the metamagnetic behavior signal the appearance of the so-called almost-localized Fermi liquid (ALFL) state, as such behavior is absent for the Landau Fermi liquid [38]. The
the presence of correlations in the sense that their presence is induced by the chemical potential, respectively. They are induced by the \( \lambda \) free-energy functional. Furthermore, the Lagrange multipliers parameter space to search for the true global minimum of the consistent equations to be obeyed, which in turn restricts the introduction of constraints results in additional self-

diminution of \( c_v \) with \( h \) is the sign of a combined decrease of both the effective-mass components, as well as of the decreasing population of the spin-minority subband.

3.2. Subsidiary quantities

The introduction of constraints results in additional self-consistent equations to be obeyed, which in turn restricts the parameter space to search for the true global minimum of the free-energy functional. Furthermore, the Lagrange multipliers \( \lambda_m \) and \( \lambda_n \) play the role of an effective field and a shift of the chemical potential, respectively. They are induced by the correlations in the sense that their presence is induced by the presence of \( q_\sigma \) and, more particularly, by its singular dependence on both \( m \) and \( n \) in the present situation. The fields \( \lambda_m \) and \( \lambda_n \) are determined within the variational/self-consistent procedure and represent the third factor distinguishing an ALFL from a LFL. For the sake of completeness, in table 1 we provide exemplary values of the relevant quantities. Note that \( \lambda_m \) almost compensates \( \mu \), and in effect we obtain the effective value of the Fermi energy for the heavy quasiparticles.

In figure 6 we plot the spin-resolved density of states for the two values of \( U = 8 \) and 18 (in units of |\( t \)|) in an applied field. The spin subbands are shifted by an amount \( h + \lambda_m \) and narrowed down asymmetrically by the spin-direction dependent factor \( q_\sigma \). In figures 7(a)–(c) we have plotted \( \lambda_m \), \( \lambda_n \), and \( \mu \), all as functions of \( h \). Furthermore, the field \( \lambda_m \) as a function of magnetization \( m \) is shown in figure 8. This effective field is a nonlinear function of both \( h \) and \( m \), and represents a relatively fast growing quantity with increasing \( h \). It is only weakly dependent on \( h \) in the moderate interaction limit. This means that the presence of \( \lambda_m \) will have an essential impact on the magnetic properties, while the relative constancy of \( \mu \) and \( \lambda_n \) in the regime \( h < h_{\text{crit}} \) explains the flat behavior of \( c_v(T) \) in that regime. It would be interesting to see if the presence of the effective field \( \lambda_m \) acting on the spin degrees of freedom only (in analogy to the Weiss molecular field) can be detected with the same accuracy as the spin splitting of the masses. Such a test would be a decisive step forward in defining an almost-localized Fermi liquid as a separate state from the Landau Fermi liquid. Note, however, that \( \lambda_m \) cannot be, strictly speaking, considered as a molecular Weiss field, since it is nonlinear in \( m \).

3.3. Concrete example: liquid\(^3\)He

Liquid \(^3\)He is regarded as a canonical example of the Landau Fermi liquid (cf. e.g. [6]). It has also been regarded as an ALFL, as it undergoes a transition to the solid state at a pressure \( p \gtrsim 34 \) bar, with the localization of the \(^3\)He atoms regarded as a fermions of spin \( \frac{1}{2} \) [9, 12, 39]. Here we briefly discuss its behavior in an applied magnetic field at ambient pressure. We have compared the magnetization curve obtained
Figure 6. Spin-resolved density of states of quasiparticle states in the applied magnetic field $h = 0.5$ for the selected values of $U$. The spin (magnetic-moment)-minority subband is narrowed, whereas the spin-majority-spin subband is widened so that it acquires the bare bandwidth as the saturation state is reached in the strong-field limit.

Table 1. Values of the parameters obtained for $U = 12, t' = 0.25, n = 0.97, \beta = 500$ (in units where $|t| = 1$) for four values of the reduced magnetic field. The calculations were made for a fcc lattice of size $200 \times 200 \times 200$.

| Quantity | $h = 0$ | $h = 0.2$ | $h = 0.5$ | $h = 1$ |
|----------|---------|-----------|-----------|---------|
| $F$      | -6.475 2954 | -6.476 5977 | -6.435 4871 | -6.051 8362 |
| $\lambda$ | 0.323 1845 | 0.319 33441 | 0.295 0449 | 0.237 0746 |
| $\mu$    | 5.838 7352 | 5.822 7839 | 5.684 5669 | 4.981 5074 |
| $\lambda_m$ | -5.574 7470 | -5.560 1127 | -5.459 9753 | -5.214 1073 |
| $\lambda_m$ | 0 | 0.400 7685 | 1.141 0240 | 2.180 9003 |
| $q_\uparrow$ | 0.725 0737 | 0.729 3968 | 0.748 2932 | 0.797 1271 |
| $q_\downarrow$ | 0.725 0737 | 0.723 6794 | 0.730 7299 | 0.756 9461 |

Figure 7. Panels (a)–(c) show the evolution of the fields $\lambda_m$ and $\lambda_n$ and the chemical potential $\mu$ with respect to the applied magnetic field. The field $\lambda_m$ appears only in the spin polarized state, whereas $\lambda_n$ is almost compensated by $\mu$.

from our model with the experimental magnetization [31] of the liquid $^3$He, as shown in figure 9. We find a good overall agreement. Note that our results, obtained for $n < 1$, do not exhibit the discontinuous metamagnetic transition which disqualified the applicability of the standard GA to $^3$He with $n = 1$ [9]. To avoid this discontinuity, we have introduced about 5% of vacancies in this virtual fcc lattice representing liquid $^3$He. This number of vacant sites provides the best fit of our results to the experimental data. Furthermore, it is important to note that the relatively small number of holes introduced preserves the almost-localized nature of this quantum liquid. This note is important also in view of the circumstance that the detailed $m(h)$ dependence is very sensitive to the number of quantum vacancies. It is tempting to suggest that the effective
empty-site content \( \delta \equiv 1 - n \) of the order of a few percent can be interpreted as the presence of quantum vacancies in the liquid state, in direct analogy to the quantum Andreev vacancies postulated and observed in solid \(^3\)He [40]. From a detailed analysis of the fitting procedure we conclude that the assumption of a non-half-filled lattice is necessary if either the GA, SGA or DMFT approaches and the Hubbard model are to emulate the magnetic behavior of liquid \(^3\)He.

One important difficulty of the just discussed results (figure 9) should be raised at this point. Namely, a relatively small value of \( U \sim 5|t| \ll W \) (where \( W \equiv 24|t| \) is the bare band width) obtained from the \( m(h) \) best fit places the liquid \(^3\)He at ambient pressure as a moderately correlated system. This seemingly unexpected conclusion is also in agreement with the DMFT analysis [21]. In this way, the Hubbard model approach also squares qualitatively with the fundamental Fermi liquid theory assumption that the interaction between quasiparticles can be essentially limited to the region very close to the Fermi surface (\( U \) substantially smaller than \( W \)). Furthermore, the method for estimating the number of vacancies might be associated with a detailed study of the field dependence of the specific heat to determine a possible spin-direction dependence of the effective mass, though the weak effect for this moderate value of \( U \) may be prove decisive. Such an explicit spin-direction mass dependence is absent when we have the exactly half-filled situation (i.e., one atom per site, without any vacant cells).

Furthermore, in spite of this success in explaining \( m(h) \) in a semiquantitative manner, there still is another problem concerning determination with the same set of parameters of a realistic value of the mass enhancement estimated from the \( c_V(T) \) curves for \( T \to 0 \) [3, 4]. Namely, the value of the specific heat enhancement at \( h = 0 \) obtained for \( U = 5|t| \sim W/5 \) is far too small to provide the corresponding effective mass enhancement \( m^* = 2.86m_0 \) at ambient pressure, where \( m_0 \) is the free \(^3\)He atomic mass. This disagreement is common to the present and the previous [12, 21] treatments. A small mass enhancement within the GA, SGA or DMFT of the mass can be interpreted in two ways. First, the spin-fluctuation contribution can be very important [41]. In that situation, the SGA should be considered only as a saddle-point approximation to a more complete approach (cf. appendix B). This question certainly requires a detailed analysis. Second, one has to note that the \( m^*/m_0 \) ratio estimate from the experimental \( c_V \) data [3, 4], based on the relations to an ideal gas, may not be fully adequate either. Finally, our assumption that \( N_e < N_L \) and \( \delta \equiv 1 - n \), independent of \( h \) or pressure, may be analyzed further as well.

4. Conclusions

We have carried out a systematic study of a correlated Fermi liquid modeled by the Hubbard model on a fcc lattice, utilizing the statistically consistent Gutzwiller approach (SGA) [42] in an applied magnetic field and in an almost-half-filled regime. Within this method, the field and spin-direction dependent effective masses, the magnetization curve, the magnetic susceptibility, and the specific heat, were all calculated in a both self-consistent and variationally optimal manner. We have found a metamagnetic-like behavior, tracing the discontinuities which would appear for the half-filled band case (one particle per cell). In other words, we have not obtained any first-order metamagnetic transition which limits the applicability of the original Gutzwiller approach (GA) to real systems such as liquid \(^3\)He (see also the discussion in [21]). Apart from that, the GA approach is not statistically consistent, as discussed in detail in the text. We have found a good overall agreement of our approach with experimental data for the magnetization of liquid \(^3\)He. However, there remains the question of putting into mutual agreement the magnetization data and the magnitude of effective mass enhancement observed for that system in zero applied field. The quantitative analysis within the lattice-approach required the introduction of a small number (~5%) of vacant cells to destroy the strong metamagnetism. A way of including the spin fluctuations is suggested (cf. appendix B), starting from the SGA state, which should then be regarded as a saddle-point state for a more complete analysis. In this manner, the SGA state replaces the Hartree–Fock state, regarded so far as a reference (saddle-point) state for further considerations concerning spatially inhomogeneous fluctuations [43–45], here of both spin and charge types.

In summary, our SGA approach, as well as the works carried within DMFT [21, 34, 35] provide a convergent quasiparticle language in the sense that the effective masses are dependent on the spin-direction in the magnetically polarized state. We also introduce a set of nonlinear effective fields, determined in a self-consistent manner, which renormalize both the chemical potential and the applied field magnitude experienced by the quasiparticles representing the almost-localized Fermi liquid. Our method of approach may be regarded as equivalent to the slave-boson approach in the saddle-point approximation [42], without involving the slave-boson fields which introduce spurious Bose-condensation phase transitions at nonzero temperature.
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Appendix A. Statistically consistent Gutzwiller approximation

As pointed out in the main text, it has been noticed (see [42, 46, 47] and references therein) that the Gutzwiller approximation which leads to the effective single-particle Hamiltonian (2) has a principal drawback. Namely, if we try to calculate the ground state energy from $E_G \equiv \langle H_{GA} \rangle$, we have first to determine the average spin polarization $m$, the double occupancy probability $d$ and等着enz. This can be achieved in two ways: either by minimizing the free-energy functional $F$ for $T \geq 0$ (defined by equation (5) for $\lambda_m = \lambda_n = 0$) with respect to the variables $(m, d^2, n)$ or by writing down the self-consistent equation of $m$ and $n$ and minimizing $F$ with respect to $d^2$. Those two procedures should provide the same answers if (2) properly represents the defined single-particle Hamiltonian. In fact, the results do differ [42, 47], and this discrepancy is caused by the fact that the single-particle energies depend on $q_\sigma$, which depends on $m$ and $n$ in a non-analytic manner (see, for example, the limits $n \rightarrow 1$ and/or $m \rightarrow 1$). The presence of this discrepancy means that the GA violates the fundamental Bogoliubov theorem, stating that the effective single-particle states represent the optimal quasiparticle states in the variational sense, with the ordinary self-consistent procedure preserved at the same time.

To cure this principal defect one can choose an approach in which one imposes the constraints so that the consistency from the point of view of statistical mechanics is preserved. To carry through such a procedure one can utilize the maximum entropy method to derive the correct statistical distribution (with constraints) and then proceed further [47]. Here we have chosen a slightly different path. Namely, we have defined the statistically consistent Gutzwiller approximation (SGA). As a result, we have to minimize $F$ given by (5) also with respect to $\lambda_m$ and $\lambda_n$, and the procedure introduces two physically relevant fields (cf. (6)) which appear only in the correlated state ($q_\sigma \ll 1$) and vanish in the small-$U$ limit, i.e., in the Hartree–Fock limit ($q_\sigma \rightarrow 1$). The last limiting situation thus represents a test for the correctness of our approach.

One should note that the SGA is essentially based on the GA, but provides additional essential consistency of the model by introducing two extra parameters into the approach. In summary, the self-consistent equations

\[
\frac{1}{T} \sum_{i,\sigma} \sigma \langle \hat{n}_{i\sigma} \rangle = \frac{1}{T} \sum_{k,\sigma} \sigma \langle \hat{n}_{k\sigma} \rangle \equiv m, \\
\frac{1}{T} \sum_{i,\sigma} \langle \hat{n}_{i\sigma} \rangle = \frac{1}{T} \sum_{k,\sigma} \langle \hat{n}_{k\sigma} \rangle \equiv n, \\
\langle \hat{n}_{k\sigma} \rangle = \delta_{k\sigma} \langle \hat{n}_{i\sigma} \rangle, \quad \frac{\sigma}{\partial \hat{n}_{k\sigma}} \rightarrow \delta_{k\sigma},
\]

are consistent with the variational equations (7) derived within the SGA method.

Appendix B. SGA as a saddle-point approximation

Here we would like to sketch the method of extending the SGA approach. In this method SGA is regarded as a saddle-point approximation to a more complete theory which includes the quantum fluctuations.

In general, the constraints in (4) should be written in the local form

\[ -\left\{ \sum_{i\sigma} \lambda_{ni} \sigma (\hat{n}_{i\sigma} - \langle \hat{n}_{i\sigma} \rangle) + \sum_{i\sigma} \lambda_{ni} (\hat{n}_{i\sigma} - \langle \hat{n}_{i\sigma} \rangle) \right\} = \sum_{i\sigma} (\lambda_{ni} \delta S_i^z - \lambda_{ni} \delta \hat{n}_{i\sigma}), \quad \text{(B.1)} \]

The last term can be rewritten in the spin explicit form

\[ \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = \left( \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow} \right)^2 + \frac{\hat{n}_{i\uparrow}^2}{2} + \frac{\hat{n}_{i\downarrow}^2}{2}, \quad \text{(B.2)} \]

where $\langle \hat{S}_i^z \rangle \equiv m$ and $\hat{n}_{i\uparrow} \equiv \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$. In effect, we have

\[ U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = U \sum_i \delta (\hat{S}_i^z)^2 + U \sum_i \frac{\hat{n}_{i\uparrow}^2}{2} + \text{const}. \quad \text{(B.3)} \]

One can reformulate the whole approach in the spin rotationally invariant form in a straightforward manner. In effect, we have linear and quadratic spin and charge fluctuations. We can thus define the part of the Hamiltonian responsible for fluctuations as

\[ \hat{H} = \hat{H}^{SGA} + \hat{H}^{\text{fluct}} + \text{const.} \quad \text{(B.4)} \]

where

\[ \hat{H}^{\text{fluct}} = -\sum_i \left[ \lambda_{ni} \delta S_i^z - \lambda_{ni} \delta \hat{n}_{i\sigma} \right] + U \sum_i (\delta S_i^z)^2 + \frac{1}{2} (\delta \hat{n}_{i\sigma})^2. \quad \text{(B.5)} \]
This expression (B.6) (or their spin-rotation invariant correspondents) should be inserted into the expression for the energy expressed in the functional-integral form over the Fermi fields [48] and then evaluated explicitly, as it involves cumbersome calculations. Methodologically, it is analogous to the slave-boson approach [41]. However, the present approach involves only coherent physical Fermi \( \hat{c}_{i\sigma} \) and Bose \( \{\lambda_m, \lambda_n\} \) fields, without introducing condensing ghost slave-boson fields.

When the reference (saddle-point) system is represented by an almost-localized Fermi liquid, both the spin and charge fluctuations thus become relevant. This should lead to a renormalization of the thermodynamic properties and should be analyzed separately, as in the present paper we concentrate on the \( T \to 0 \) results. Nonetheless, inclusion of the fluctuations should lead to a further enhancement of the specific heat, as well as to the presence of the \( T^3 \ln T \) term for \( h = 0 \) [41].

References

[1] Landau L 1956 Zh. Exp. Teor. Fiz. 30 1058
Landau L 1957 Sov. Phys.—JETP 3 920 (Engl. transl.)
[2] Landau L 1957 Zh. Exp. Teor. Fiz. 32 59
Landau L 1957 Sov. Phys.—JETP 5 101 (Engl. transl.)
[3] Greywall D S 1983 Phys. Rev. B 27 2747
[4] Greywall D S 1986 Phys. Rev. B 33 7520
[5] Mook H A 1985 Phys. Rev. Lett. 55 2452
[6] Dobbs E 2000 Helium Three (Oxford: Oxford University Press)
[7] Gebhard F 1997 The Mott Metal-Insulator Transitions (Berlin: Springer)
[8] Spalek J and Gopalan P 1990 Phys. Rev. Lett. 64 2823
[9] Vollhardt D 1984 Rev. Mod. Phys. 56 99
[10] Castorina P, Gavani R V and Satz H 2010 Eur. Phys. J. C 69 169
[11] Satz H 2012 Acta Phys. Pol. B 43 587
[12] Vollhardt D, Wölfle P and Anderson P W 1987 Phys. Rev. B 35 6703
[13] Scalapino D J 2012 Rev. Mod. Phys. 84 1383
[14] Jędrak J and Spalek J 2011 Phys. Rev. B 83 104512
[15] Bünenmann J, Schickling T and Gebhard F 2012 Europhys. Lett. 98 27006
[16] Kaczmarczyk J, Spalek J, Schickling T and Bünenmann J 2013 Phys. Rev. B 88 115127
[17] Gutzwiller M 1965 Phys. Rev. 137 A1726
[18] Bünenmann J, Gebhard F and Thul R 2003 Phys. Rev. B 67 075103
[19] Spalek J 1990 J. Solid State Chem. 88 70
[20] Brinkman W F and Rice T M 1970 Phys. Rev. B 2 4302
[21] Parihari D, Vidhyadhararaj N S and Taraphder A 2011 J. Phys.: Condens. Matter 23 055602
[22] Jarrell M 1992 Phys. Rev. Lett. 69 168
[23] Jędrak J and Spalek J 2010 Phys. Rev. B 81 073108
[24] Kaczmarczyk J and Spalek J 2011 Phys. Rev. B 84 125140
[25] Abram M, Kaczmarczyk J, Jędrak J and Spalek J 2013 Phys. Rev. B 88 094502
[26] Howczak O and Spalek J 2012 J. Phys.: Condens. Matter 24 205602
[27] Spalek J, Datta A and Honig M 1987 Phys. Rev. Lett. 59 728
[28] Spalek J, Kokosowski M and Honig J M 1989 Phys. Rev. B 39 4175
[29] Spalek J 2005 Physica B 365 378
[30] Spalek J 2006 Phys. Status Solidi b 243
[31] Wiegers S A J, Wolf P E and Puech L 1991 Phys. Rev. Lett. 66 2895
[32] 0954612078Galassi M, Davies J, Theiler J, Gough B, Jungman G, Alken P, Booth M and Rossi F GNU Scientific Library Reference Manual 3rd edn
[33] Maška M, Mierzejewski M, Kaczmarczyk J and Spalek J 2010 Phys. Rev. B 82 054509
[34] Bauer J and Hewson A C 2007 Phys. Rev. B 76 035118
[35] Bauer J 2009 Eur. Phys. J. B 68 201
[36] McCollam A, Julian S R, Rourke P M C, Aoki D and Flouquet J 2005 Phys. Rev. Lett. 94 186401
[37] Sheikin J, Groger A, Raymond S, Jaccard D, Aoki D, Harima H and Flouquet J 2003 Phys. Rev. B 67 094420
[38] Korbel P, Spalek J, Wójcik W and Acquarone M 1995 Phys. Rev. B 52 R2213
[39] Spalek J 2000 Eur. J. Phys. 21 511
[40] Andreev A 1976 Zh. Eksp. Teor. Fiz. 24 608
Andreev A 1976 JETP Lett. 24 564 (Engl. transl.)
[41] Wolfle P and Li T 1990 Z. Phys. B 78 45
[42] Jędrak J, Kaczmarczyk J and Spalek J 2010 (arXiv:1008.0021)
[43] Hertz J 1976 Phys. Rev. B 14 1165
[44] Moriya T 1985 Spin Fluctuations in Itinerant Electron Magnetism (Berlin: Springer)
[45] Millis A J 1993 Phys. Rev. B 48 7183
[46] Wysokiński M, Jędrak J, Kaczmarczyk J and Spalek J 2012 AIP Conf. Proc. 1485 319
[47] Jędrak J 2011 Real-space pairing in an extended J=J model PhD Thesis Jagiellonian University, Kraków
[48] Spalek J 2012 Acta Phys. Pol. A 121 764 (cf. Appendix E)