Almost Localized Fermions and Mott-Hubbard Transitions at Non-Zero Temperature

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Abstract. We summarize a mean-field picture of the quasiparticle states of almost localized fermions and the first-order metal-insulator transitions at nonzero temperature, as well as make a comparison between theory and experiment for pure and doped $V_2O_3$ systems. We also discuss some of the unresolved questions for almost localized fermions such as the spin dependence of the effective mass, the metamagnetism and the instability of the Fermi surface at the Mott localization boundary.

1. Introduction

The almost localized or Mott-Hubbard fermion systems are the metallic systems for which their band energy $E_B < 0$ is comparable in magnitude to the energy $E_C > 0$ of the Coulomb interaction between the particles. In effect, the metallic phase (often called an almost localized Fermi liquid, ALFL) transforms into an antiferromagnetic (Mott) insulator under a relatively small changes in either temperature, alloy composition or pressure. This almost localized electron liquid is characterized by an enhanced value of the effective mass $m^*$, with the ratio $m^*/m_0$ in the range $2 - 10$, by a large $T^2$ term in resistivity at temperatures $T < 10K$, by the presence of the $T^3\ln T$ term in the specific heat in some systems, and by the presence of an antiferromagnetic ordering in the metallic phase, with a small magnetic moment. Furthermore, the absence of the ferromagnetic correlations in the metallic phase means that the linear specific heat coefficient ($\gamma$) and low-T magnetic susceptibility ($\chi$) enhancement factors, $\gamma/\gamma_0$ and $\chi/\chi_0$, are within the same order of magnitude so that the dimensionless Wilson ratio $R = (\chi/\chi_0)/(\gamma/\gamma_0)$ is in the range $1 < R \leq 4$. Most of the above features of ALFL phase are also shared by the heavy fermion systems, although in the latter case the enhancement factors are $1 - 2$ orders of magnitude larger.

From the theoretical point of view the first question is whether almost localized fermion systems represent a separate universality class of fermion liquid or whether there is a continuous evolution from the Landau Fermi liquid (LFL) to the ALFL state, which terminates at the Mott localization boundary. In the mean-field picture the evolution LFL $\rightarrow$ ALFL in zero applied field is
gradual. The second question addresses the nature of the Mott-Hubbard transition, which in the canonical cases of pure and doped \( V_2O_3 \) and \( NiS_{2-\varepsilon}Se_\varepsilon \) is almost always of the first order. Simply phrased, the problem is in envisaging how a thermal stimulus of 100K (or 10meV) can induced radical changes in the nature of electronic states (disappearance of the Fermi surface!) on the scale of electronvolts. It turns out that in those systems the compensation \( E_C + E_B \approx 0 \) makes much smaller entropic (thermal) or atomic disorder or pressure contributions to the total free energy prominent, making in turn possible qualitative changes in the nature of the many-particle state [1].

In this paper we derive first the Gutzwiller-Brinkman-Rice picture of ALFL for quasiparticles, within the modified version [2] of slave boson approach, which is rotationally invariant in the spin space [3,4]. This derivation will be followed up by a detailed discussion of quasiparticle states and our earlier results for the Mott-Hubbard transitions at finite temperature [1,5]. Similar results were obtained recently in the limit of infinite dimensions [6]. Finally, we discuss some unobserved as yet properties of almost localized fermions such as the magnetic field dependence of effective mass \( (m^* = m_\text{g}) \) and of \( \gamma \), metamagnetism, as well as the instability of the Fermi surface.

2. Quasiparticle picture of almost localized fermions

2.1. Rotationally invariant slave boson approach

In the slave boson approach we start from the atomic (Wannier) representation of fermion states on i-th lattice site. For the case of one orbital per site the basis is composed of four states \( |0, i>, |\sigma, i> = a_{i\sigma}^\dagger |0>, i> \), and \( |2, i> = \sigma a_{i\sigma}^\dagger a_{i\bar{\sigma}}^\dagger |0>, i> \). They correspond to empty, singly occupied state with spin \( \sigma = \pm 1 \), and the doubly occupied configuration, respectively. These state are represented as follows

\[
|0, i> = \epsilon_i^\dagger |v>, \\
|1, i> = P_i^\dagger f_i^\dagger |v>, \\
|2, i> = \sigma d_i^\dagger f_i\sigma^\dagger f_i\bar{\sigma}^\dagger |v>,
\]

where \( f_i^\dagger \equiv \{f_{i\uparrow}^\dagger, f_{i\downarrow}^\dagger\} \) is the spinor pseudofermion field and \( P_i^\dagger \) is a 2 x 2 matrix

\[
P_i^\dagger \equiv a \ p_{i0}^\dagger 1 + b \ p_i^\dagger \tau,
\]

containing four Bose fields \( p_{i0}^\dagger \) and \( p_i^\dagger \equiv (p_{i\uparrow}^\dagger, p_{i\downarrow}^\dagger, p_{i\bar{\sigma}}^\dagger) \), in addition to the fields \( \epsilon_i^\dagger \) and \( d_i^\dagger \) of the same type. \( \tau = (\tau_x, \tau_y, \tau_z) \) are the Pauli matrices. The normalization constants are determined from the fundamental commutation relations for the matrix \( P_i^\dagger \) and its components, which are