Perturbative approach to three-component fermionic atoms in optical lattices

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Abstract. We develop a perturbative approach combined with the dynamical mean-field theory for investigating the Mott transition in repulsively interacting three-component fermionic atoms in optical lattices. We show that this method captures the essentials of the correlation effects and describes well the crossover between the Fermi liquid and the paired Mott insulator.

The high controllability of cold atoms in optical lattices enables us to investigate quantum many-body effects that cannot be observed in condensed matter physics [1, 2, 3]. Recently, degenerate gases of three-component (color degree of freedom) $^6$Li fermions have been successfully created and their novel features have been revealed [4, 5]. For three-component repulsive fermionic atoms in optical lattices by using the self-energy functional approach (SFA) we showed that a paired Mott insulator (PMI) appears at half filling, although the average atom number per site is non-integer $3/2$ [6, 7]. When two of the three repulsions between different two-color atoms are stronger than the other, effective pairs of weakly repulsing atoms are formed to avoid the stronger two repulsions. Accordingly, in a PMI the effective particle number at a site becomes an integer [7]. In this system, other phase transitions accompanied by symmetry breaking are possible such as a color density wave [6, 8, 9] and a color selective antiferromagnet [6]. For attractively interacting systems, it was shown that a color superfluid appears [10, 11]. To investigate these characteristic phase transitions, we require another method complementary to the SFA. A Feynman diagrammatic approach combined with the dynamical mean-field theory (DMFT) can be an efficient method. This method is called the iterated perturbation theory (IPT), and it has been applied successfully to various types of phase transitions [12, 13]. The diagrammatic approaches have provided us with rich knowledge on the scattering processes relevant to the various phase transitions. Furthermore, the IPT consumes few computational resources. Therefore, the IPT helps us to carry out systematic calculations that capture the essentials of the phase transitions.

In this paper, we develop the IPT by modifying straightforward perturbative calculations. We apply this method to the phase transition/crossover between a Fermi liquid (FL) and a PMI. We compare the results with those obtained with unperturbative calculations using the SFA [6, 7]. We discuss the validity of our approach.

The low-energy properties of repulsively interacting three-component fermionic atoms in
optical lattices are well described by the following Hubbard-type Hamiltonian:

\[ \hat{H} = -t \sum_{\langle i,j \rangle} \sum_{\alpha=1}^{3} \hat{a}_{i\alpha}^{\dagger} \hat{a}_{j\alpha} - \sum_{i} \mu_{\alpha} \hat{n}_{i\alpha} + \frac{1}{2} \sum_{i} \sum_{\alpha \neq \beta} U_{\alpha\beta} \hat{n}_{i\alpha} \hat{n}_{i\beta}, \]

where the subscript \( \langle i,j \rangle \) is the summation over the nearest-neighbor sites, and \( \hat{a}_{i\alpha}^{\dagger} (\hat{a}_{i\alpha}) \) and \( \hat{n}_{i\alpha} \) are creation (annihilation) and number operators of a fermion with color \( \alpha \) at the \( i \)th site. Here, \( t \) denotes the hopping integral and \( \mu_{\alpha} \) is the chemical potential for an atom with color \( \alpha \). By choosing \( \mu_{\alpha} \) adequately, atoms with each color achieve a balanced filling \( n_{\alpha} \). We set \( U_{12} \equiv U \) and \( U_{23} = U_{31} \equiv U' \), and introduce an anisotropy ratio \( R \equiv U/U' < 1 \). We neglect the confinement potential for the first approximation.

To investigate the phase transition driven by the local correlation effects, we consider an infinite dimensional system, which is a nontrivial limit for discussing the Mott insulator [12]. According to the DMFT [12] the self-energy \( \Sigma_{\alpha}(i\omega_n) \) is purely local and independent of the wave number \( q \). The self-energy \( \Sigma_{\alpha}(i\omega_n) \) is obtained from the effective impurity model, whose Hamiltonian is

\[ \hat{H}_{\text{imp}} = \sum_{\alpha=1}^{3} \varepsilon_{\alpha} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\alpha} - \sum_{\alpha=1}^{3} \mu_{\alpha} \hat{n}_{\alpha} + \sum_{\alpha=1}^{3} \sum_{q} \left[ V_{q\alpha} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\alpha} + \text{c.c.} \right] + \frac{1}{2} \sum_{\alpha \neq \beta} U_{\alpha\beta} \hat{n}_{\alpha} \hat{n}_{\beta}, \]

where \( \hat{n}_{\alpha} = \hat{d}_{\alpha}^{\dagger} \hat{d}_{\alpha} \). We introduce the cavity Green’s function \( g_{\alpha\alpha}(i\omega_n) \) corresponding to the non-interacting impurity Green’s function, which satisfies the Dyson equation \( g_{\alpha\alpha}(i\omega_n) = [g_{\alpha\alpha}^{-1}(i\omega_n) - \Sigma_{\alpha}(i\omega_n)]^{-1} \). The impurity Green’s function \( g_{\alpha\alpha}(i\omega_n) \) has to be equal to the local Green’s function \( G_{\alpha\alpha}(i\omega_n) = \frac{\pi}{\omega} g_{\alpha\alpha}(i\omega_n, \mathbf{q}) \). In this way, the DMFT self-consistent loop is completed. We approximate the self-energy from the first- and second-order contributions. The first-order contributions are given by \( \Sigma_{\alpha}^{(1)}(= \Sigma_{\alpha}^{(1)} = U' n_3 \) and \( \Sigma_{\alpha}^{(2)} = U' n_1 + U' n_2 \). The second-order contributions are given by \( \Sigma_{\alpha}^{(2)}(i\omega_n) = \Sigma_{\alpha}^{(2)}(i\omega_n) = \sum_{l} [U' g_{\alpha}(i\omega_n + i\nu_{l}) \chi_{\alpha}(i\nu_{l}) + U g_{\alpha}(i\omega_n + i\nu_{l}) \chi_{\alpha}(i\nu_{l})] \) and \( \Sigma_{\alpha}^{(2)}(i\omega_n) = \sum_{l} [2 U g_{\alpha}(i\omega_n + i\nu_{l}) \chi_{\alpha}(i\nu_{l})] \), where \( \chi_{\alpha}(i\nu_{l}) = -\sum_{n} g_{\alpha}(i\omega_n + i\nu_{l}) g_{\alpha}(i\omega_n) \).

We modify the self-energy as \( \Sigma_{\alpha} = \Sigma_{\alpha}^{(1)} + A_{\alpha} \Sigma_{\alpha}^{(2)} \) by introducing the prefactor \( A_{\alpha} \). This kind of the prefactor was successfully introduced for investigating the crossover from BCS superconductivity to Bose-Einstein condensation in the attractive Hubbard model [13]. To determine the prefactor \( A_{\alpha} \), we perform a momentum expansion of \( G_{\alpha\alpha}(i\omega_n) \) in the power of \( 1/\omega \) for \( \omega \to \infty \),

\[ G_{\alpha\alpha}(i\omega_n) = \frac{\langle \{ \hat{d}_{\alpha}, \hat{d}_{\alpha}^{\dagger} \} \rangle}{\omega} + \left\{ \langle \{ \hat{d}_{\alpha}, \hat{H}_{\text{imp}}, \hat{d}_{\alpha}^{\dagger} \} \rangle / \omega^2 + \langle \{ \hat{d}_{\alpha}, \hat{H}_{\text{imp}}, \hat{d}_{\alpha}^{\dagger} \} \rangle / \omega^3 \right\} + \ldots \]

where \( \{ , \} \) and \( \{ , \} \) denote the commutator and anticommutator, respectively, and \( D_{\alpha\beta} = \langle n_{\alpha} n_{\beta} \rangle \) is the double occupancy obtained from \( D_{\alpha\beta} = -\sum_{\gamma} \text{tr} \{ G_{\gamma \gamma} \hat{H} \hat{d}_{\alpha\beta} \} \). From the Dyson equation \( \Sigma_{\alpha}(i\omega_n) = g_{\alpha\alpha}^{-1}(i\omega_n) - G_{\alpha\alpha}^{-1}(i\omega_n) \) and Eq. (3), we obtain an exact expression for the self-energy \( \Sigma_{\alpha}(i\omega_n) \). For instance, we obtain the exact expression as \( \Sigma_{\beta}(\omega) = \langle 2 U^2 n_1 (1 - n_1) + 2 U^2 (D_{12} - n_1 n_2) \rangle / \omega + \ldots \), while the perturbative expression is
Figure 1. (Color Online) Renormalization factor $Z_\alpha$ and double occupancy $D_{\alpha\beta}$ calculated (a) by including the prefactor $A_\alpha$, (b) without including it ($A_\alpha = 1$), and (c) by using the SFA as functions of $U'/t$ for $R = 0.1$ and $T/t = 0.1$ at half filling.

Figure 2. (Color Online) (a) Prefactor $A_\alpha$ as a function of $U'/t$ for $U/t = 3$, $R = 0.1$, and $T/t = 0.01$ at half filling.

$$\Sigma_3^{(2)}(\omega) = 2U'^2n_{c1}(1 - n_{c1})/\omega + \cdots.$$ Comparing the two expressions, we obtain the prefactors $A_\alpha$ as

$$A_1 = A_2 = \frac{U'^2n_1(1 - n_2) + U'^2n_2(1 - n_3) + 2UU'(D_{23} - n_2n_3)}{U'^2(n_{c2}(1 - n_{c2}) + U'^2n_{c3}(1 - n_{c3})}, \quad (4)$$

$$A_3 = \frac{n_1(1 - n_1) + D_{12} - n_1n_2}{n_{c1}(1 - n_{c1})}, \quad (5)$$

where $n_{c\alpha} = \sum_i g_\alpha(i\omega_n)e^{i\omega_n}/\omega_0$.

On the basis of this IPT, we calculate the renormalization factor $Z_\alpha \equiv 1/[1 - \text{Im}[\Sigma_\alpha(i\pi T) - \Sigma_\alpha(-i\pi T)]/2\pi T]$ [14] and the double occupancy $D_{\alpha\beta}$. For noninteracting atoms, we use a semicircular density of states, $\rho_0(x) = \sqrt{4t^2 - x^2}/(2\pi t^2)$. We also perform unperturbative calculations using the SFA. We compare both results and discuss the validity of this IPT.

In Fig. 1, we show the $U'/t$ dependence of $D_{\alpha\beta}$ and $Z_\alpha$ for $R = 0.1$ and $T/t = 0.1$ at half filling. Figure 1(a), (b), and (c) show the results obtained by including the prefactor $A_\alpha$, without it ($A_\alpha = 1$), and by using the SFA, respectively. Since we set $U_{12} \equiv U$ and $U_{23} = U_{31} \equiv U'$, $Z_1 = Z_2$ and $D_{23} = D_{31}$. As $U'/t$ increases, $Z_\alpha$ decreases and approaches zero asymptotically,
indicating that there is a crossover from the FL to the Mott insulator. By extrapolating $Z_\alpha$ from small $U'/t$, we find that $Z_1$ and $Z_3$ become zero at the same $U'/t$. The crossover points thus obtained are evaluated to be $U'/t = 4.0, 4.1,$ and $2.8$ in Fig. 1(a), (b), and (c), respectively. In Fig. 1(a) and (c), $D_{12}$ ($D_{13}$) increases (decreases) towards 0.5 (zero), as $U'/t$ increases. The results show that paired color-1 and -2 atoms are formed in the Mott insulating phase. This is consistent with the fact that the renormalization effects of color-3 atoms are stronger than those of color-1 and -2 atoms ($Z_3 < Z_1$). In Fig. 1(a) and (c), the $U'/t$ dependences of $Z_\alpha$ and $D_{\alpha\beta}$ are qualitatively the same. In particular, the double occupancies well describe the situation for the appearance of the PMI, in that the stronger $U'$ is avoided. On the other hand, in Fig. 1(b) both $D_{12}$ and $D_{13}$ decrease and maintain finite values with increasing $U'/t$. It is difficult to picture the Mott insulating state based on this result. Therefore, we argue that the modified self-energy that results from the inclusion of $\Sigma_\alpha$ captures the essentials of the correlation effects and well describes the PMI transition/crossover.

In Fig. 2, we show the $U'/t$ dependence of the prefactor $A_\alpha$ for $R = 0.1$ and $T/t = 0.1$ at half filling. As $U'/t$ increases, $A_3$ increases and $A_1$ decreases. The results indicate that the effective interaction of color-1 and -2 atoms decreases, while that of color-3 atoms increases. These features occur because the color-1 and -2 atoms form effective pairs to avoid the strong repulsions from color-3 atoms.

In summary, we have shown that our modified IPT captures the essentials of the correlation effects and well describes the FL-PMI transition/crossover. Close to the PMI transition point, we expect superfluid pair fluctuations to be strongly enhanced. Therefore, the superfluid transition can occur in spite of the repulsively interacting atoms. The present IPT is efficient for studying the superfluid transition in repulsively interacting three-component fermionic atoms in optical lattices. The results will be published elsewhere [15]. We finally remark on a possible application of the present IPT method to translational symmetry breaking states such as the density wave state. We can analyze these states by dividing the lattice into sublattices and then slightly modifying our IPT formulation.

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