Quantum phases of Bose-Fermi mixtures in optical lattices

K. Noda\textsuperscript{a}, R. Peters\textsuperscript{a}, N. Kawakami\textsuperscript{a}, and Th. Pruschke\textsuperscript{b}

\textsuperscript{a}Department of Physics, Kyoto University, Kyoto 606-8502, Japan
\textsuperscript{b}Institut für Theoretische Physik, Universität Göttingen, Göttingen D-37077, Germany

E-mail: noda@scphys.kyoto-u.ac.jp

Abstract. We consider a mixture of interacting bosons and fermions in optical lattices described by the Bose-Fermi Hubbard Hamiltonian. To treat bosonic degrees of freedom, we use a generalized dynamical mean field theory (GDMFT). By combining the GDMFT with the numerical renormalization group method, we revisit the zero-temperature phase diagram with particular emphasis on many-body effects in a supersolid state and discuss the origin of an anomalous peak structure emerging in the density of states for fermions.

Recently, systems of correlated atoms in optical lattices have attracted much interest\cite{1}. In these systems, one can tune the interaction strength by the magnetic field dependence of Feshbach resonances, and thereby simulate typical models used to study quantum many-body physics. Furthermore, the discovery of Feshbach resonances in a mixture of fermions and bosons, $^6\text{Li} - ^{23}\text{Na}$ \cite{2}, $^{40}\text{K} - ^{87}\text{Rb}$ \cite{3, 4, 5}, and $^6\text{Li} - ^{87}\text{Rb}$ \cite{6}, creates a new route to realizing a physical system without any analog in the conventional condensed matter field. Motivated by this, we consider a mixture of interacting bosons and fermions in optical lattices described by the Bose-Fermi Hubbard Hamiltonian. Preceding studies of this system have revealed the possibility of various fascinating states, such as a supersolid state \cite{7, 8, 9, 10, 11}, where a superfluid state coexists with a density wave state, or $s$-wave and $d$-wave pairing superfluid states \cite{12, 13, 14, 15, 16}, etc. A particularly interesting point raised for the supersolid state is that an unusual peak structure emerges in the density of states (DOS) for fermions near the Fermi surface \cite{10}. Here, we revisit this problem, and point out that the peak structure is related to a single-fermion excitation that is strongly renormalized by low-energy bosonic excitations, the origin of which is quite similar to that for heavy fermions in the Fermi liquid state.

We consider a mixture of spin-polarized fermions and bosons in an optical lattice system, which may be described by the following Bose-Fermi Hubbard Hamiltonian,

\[ H = \sum_{\langle i,j \rangle} (\hat{t}^b - \mu^b \delta_{ij}) \hat{b}_i \hat{b}_j + \sum_i \frac{U_b}{2} n_i^b (n_i^b - 1) + \sum_{\langle i,j \rangle} (\hat{t}^f - \mu^f \delta_{ij}) \hat{c}_i \hat{c}_j + \sum_i U_{bf} n_i^b n_i^f, \]  

where $\hat{b}_i$ ($\hat{c}_i$) annihilates a boson (fermion) at $i$th site, $n_i^b = \hat{b}_i \hat{b}_i^\dagger$ ($n_i^f = \hat{c}_i \hat{c}_i^\dagger$) represents the number operator for bosons (fermions). $\hat{t}^b(\hat{t}^f)$ is the hopping integral between the nearest-neighbor sites, $\mu^b(\mu^f)$ the chemical potential for bosons (fermions), and $U_b$ ($U_{bf}$) the on-site boson-boson (fermion-boson) interaction, respectively. $\langle i,j \rangle$ denotes summation over nearest-neighbor sites.
To treat bosonic degrees of freedom, we use a generalized dynamical mean field theory (GDMFT) introduced by several groups [9, 10, 17], where fermions are treated by dynamical mean field theory [18, 19] while the condensate fraction of bosons is treated by conventional static mean field theory. We perform the calculation using a semi-elliptic DOS $\rho(\omega) = 2/\pi \sqrt{1 - (\omega/D)^2}$ with a half bandwidth $D$. Here, the half bandwidth $D$ is given by $D = 2\sqrt{\pi}f$. In the following, we take $D$ as the energy unit.

In order to discuss the supersolid phase with long range orders, we introduce a generalized single impurity Anderson model with a two-sublattice structure. The corresponding Hamiltonian is

$$
H_{\text{GSIAM}} = \sum_{\alpha = \pm 1} \left[ -zt_b(\varphi^\dagger_{\alpha} b_{\alpha} + \varphi b_{\alpha}) + \frac{U_b}{2} n^b_{\alpha} (n^b_{\alpha} - 1) - \mu_b n^b_{\alpha} 
- \mu_f n^f_{\alpha} + \sum_k \{\epsilon_k a^\dagger_{k\alpha} a_{k\alpha} + V_{k\alpha} (c^\dagger_{\alpha} a_{k\alpha} + \text{h.c.})\} + U_{bf} n^b_{\alpha} n^f_{\alpha} \right],
$$

where $\alpha = \pm 1$ represents the sublattice index, $z$ the coordination number, $\varphi_{\alpha} = \langle b_{\alpha} \rangle$ the superfluid order parameter, and $V_{k\alpha}$ the hybridization. Following the study in Ref. [10], we use Wilson’s numerical renormalization group (NRG) [20, 21] to solve the effective impurity model, which provides reliable results in the low energy regime. This method has already been extended to include bosonic degrees of freedom [9], which enables us to calculate the superfluid order parameter $\varphi = \langle b \rangle$ and the self energy $\Sigma(\omega)$ for fermions. Note that in the framework of our two-sublattice GDMFT, we can only treat a commensurate density wave order, so that the possibility of long-period density wave order is not addressed in this paper.

We present the results obtained under the condition $zt_b = 0.05$ and $U_b = 1.0$ with fixed filling $n^f = 1/2$ for fermions and $n^b = 5/2$, where we define $n^b = \sum_{\alpha = \pm 1} \langle n^b_{\alpha} \rangle / 2$, etc. This choice of parameter turns out to be complementary to the study in Ref. [10] ($n^f = 1/2$ and $n^b = 3/2$).

By systematically calculating the DOS for fermions, $\rho(\omega)$, for several values of the fermion-boson interaction $U_{bf}$, we wish to elucidate the many-body nature emerging in the supersolid state. When $U_{bf} \neq 0$, there is always a finite amplitude of density-wave order parameter $\Delta N^f(\omega) (= 1/2|n^f_{\alpha} - n^f_{-\alpha}|) \neq 0$ both for fermions and bosons, whose density wave oscillations are out of phase, implying that the supersolid state can be realized when $\varphi \neq 0$. Actually, as $U_{bf}$ is increased, bosons can become itinerant and the supersolid state is further stabilized [10]. We here focus on the supersolid region where $1/2 < \Delta N^b < 3/2$ corresponding to $1.7 \simeq U_{bf} \simeq 2.4$.

In this region, the system has gapless (compressible) boson density fluctuations, which trigger the emergence of the superfluidity for bosons. This simultaneously gives rise to an unusual peak near the Fermi level in the DOS for fermions, as shown in Fig. 1. Titvinidze et al. [10] pointed out that the peak formation in the DOS in the supersolid phase may be related to the instability to breaking the alternating boson-fermion density wave order. We here argue that this peak

![Figure 1](image_url)

**Figure 1.** (Color online) Density of states in a supersolid state for $U_{bf}/D = 1.8, 1.9, 2.0, 2.2$. The inset shows the region near the Fermi surface.
Fermi-Bose mixture system, the fermion sector is always insulating, so that the renormalization effect due to gapless bosonic degrees of freedom (or \textit{in condensed matter physics}; when few holes are doped into a Mott insulating phase of the Hubbard model (or \textit{t-J} model) at half filling, the DOS acquires a sharp peak structure, which is caused by the renormalization effect due to mobile correlated electrons (or holes). In the present Fermi-Bose mixture system, the fermion sector is always insulating, so that the renormalization effect should be dynamically generated, so that it should be due to the fermion-boson coupling term. This implies that the peak in the fermionic DOS is induced by the fermion-boson coupling term. In order to confirm this, we systematically investigate how the shape of the peak changes according to the gapless bosonic excitations (see Fig. 1). We also show the real part of the self-energy for fermions in Fig. 2 and the density fluctuations of bosons in Fig. 3. As the interaction \( U_{fb} \) increases from 1.7, the latter quantity increases, takes maximum values, and then decreases to zero when the system approaches another insulating state around \( U_{fb} \approx 2.4 \). Accordingly, the self-energy in Fig. 2 develops a sharp structure around \( \omega = 0 \), giving rise to the peak in the fermionic DOS in Fig. 1. Note that the width of the peak becomes very sharp, while its weight once increases and then decreases, as seen in Fig. 1. This can be explained as follows. Around \( U_{fb} \sim 1.7 \), the number of effective gapless bosons is small, so that the effective interaction between bosons is not so strong, providing only the weak renormalization effect to an excited fermion. On the other hand, when \( U_{fb} \approx 2.4 \), low-energy bosons are highly correlated since the system is close to the insulating phase. These results in a strong renormalization effect for fermionic excitations, giving rise to the very sharp peak structure. We have also checked that essentially the same tendency appears in the parameters regime studied in Ref. [10].

Recall that a quite similar behaviour appears ubiquitously in correlated electron systems in condensed matter physics; when few holes are doped into a Mott insulating phase of the Hubbard model (or \textit{t-J} model) at half filling, the DOS acquires a sharp peak structure, which is caused by the renormalization effect due to mobile correlated electrons (or holes). In the present Fermi-Bose mixture system, the fermion sector is always insulating, so that the renormalization effect...
effect on one-particle excitations is unusual in the sense of ordinary electron systems. We note, however, that there is another massless boson degree of freedom in our case, which may be a source of the renormalization effect. In this sense, the peak formation in the DOS for fermions in the supersolid states may be regarded as a unique many-body effect inherent in mixed Fermi-Bose systems. In contrast to ordinary heavy fermion systems, the fermion sector in our model is in an insulating state, so that the DOS should vanish inside the charge excitation gap, resulting in the decrease in the DOS near the gap edge. This is why the anomalous peak, which is caused by massless bosonic excitations, is formed a little bit below the lower edge of the charge gap.

In summary, we have reexamined the ground state properties of a mixed Bose-Fermi system with particular emphasis on many-body effects in the supersolid phase. By examining the anomalous peak structure in the DOS for fermions, we have elucidated that it indeed comes from many body effects; while the high-energy hump structure in the DOS is dominated by the mean-field type effect of the fermion-boson interaction, the low-energy peak structure is induced by the density fluctuations of bosons through the fermion-boson interaction term. The formation of the low-energy peak is quite similar to that for heavy fermions in the Fermi liquid state. In the present case, the low-energy bosonic excitations provide a source of the strong renormalization.

Acknowledgements

This work is supported by the Grant-in-Aid for Scientific Research [Grant nos. 21540359, 20029013, 20102008] and the Global COE Program “The Next Generation of Physics, Spun from Universality and Emergence” from MEXT of Japan. N.K. is supported by the Japan Society for the Promotion of Science (JSPS) through its FIRST Program. R.P. acknowledges support from the Alexander von Humboldt Foundation and JSPS under Program “FY2010 JSPS Postdoctoral Fellowship for Foreign Researchers”. T.P. and K.N. acknowledge support by the German Science Foundation (DFG) through the SFB 602. Part of the computations were done at the Supercomputer Center at the Institute for Solid State Physics, University of Tokyo and Yukawa Institute Computer Facility.

References

[1] Bloch I, Dalibard J and Zwerger W 2008 Rev. Mod. Phys. 80 885
[2] Stan C A, Zwierlein M W, Schunck C H, Raupach S M F and Ketterle W 2004 Phys. Rev. Lett. 93 143001
[3] Inouye S, Goldwin J, Olsen M L, Ticknor C, Bohn J L and Jin D S 2004 Phys. Rev. Lett. 93 183201
[4] Ospelkaus S, Ospelkaus C, Humbert L, Sengstock K and Bongs K 2006 Phys. Rev. Lett. 97 120403
[5] Zaccanti M, D’Errico C, Ferlaino F, Roati G, Inguscio M and Modugno G 2006 Phys. Rev. A 74 041605
[6] Deh B, Marzok C, Zimmermann C and Courteille P W 2008 Phys. Rev. A 77 010701
[7] Bühler H P and Blatter G 2003 Phys. Rev. Lett. 91 130404
[8] Hebert F, Batrouni G G, Roy X and Rousseau V G 2008 Phys. Rev. B 78 184505
[9] Titvinidze I, Snoek M and Hofstetter W 2008 Phys. Rev. Lett. 100 100401
[10] Titvinidze I, Snoek M and Hofstetter W 2009 Phys. Rev. B 79 144506
[11] Orth P P, Bergman D L and Hur K L 2009 Phys. Rev. A 80 023624
[12] Illuminati F and Albus A 2004 Phys. Rev. Lett. 93 090406
[13] Wang D W, Lu¨ kin M D and Demler E 2005 Phys. Rev. A 72 051604
[14] Mathey L, Tsai W S and Neto A H C 2006 Phys. Rev. Lett. 97 030601
[15] Kliromonos F D and Tsai S W 2007 Phys. Rev. Lett. 99 100401
[16] Zajac A, Baldwin A, Scalettar R T, Rousseau V G, Denteneer P J H and Rigol M 2008 Phys. Rev. A 78 033619
[17] Byczuk K and Vollhardt D 2009 Ann. Phys. 18 622
[18] Metzner W and Vollhardt D 1989 Phys. Rev. Lett. 62 324
[19] Georges A, Kotliar G, Krauth W and Rozenberg M J 1996 Rev. Mod. Phys. 68 13
[20] Wilson K G 1975 Rev. Mod. Phys. 47 773
[21] Bulla R, Costi T A and Pruschke T 2008 Rev. Mod. Phys. 80 395