How the effective boson-boson interaction works in Bose-Fermi mixtures in periodic geometries

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We study mixtures of spinless bosons and not spin-polarized fermions loaded in two dimensional optical lattices. We approach the problem of the ground state stability within the framework of the linear response theory; by the mean of an iterative procedure, we are able to obtain a relation for the dependence of boson-boson effective interaction on the absolute temperature of the sample. Proceeding from such a formula, we write down analytical expressions for Supersolid (SS) and Phase Separation (PS) transition temperatures, and plot the phase diagrams.

I. INTRODUCTION

The possibility to achieve very low temperatures and the feasibility in the laboratory of implementing optical lattices represent the proper arena where testing the validity of certain condensed-matter theories and observing the manifestations of effects related to quantum mechanical statistics. Within the interesting interplay between quantum atom optics and condensed matter physics, recent trends are study of the superfluid to Mott-insulator phase transition in bosonic systems, (see [1] and [2]), and the striving for the realization of a BCS-type condensate in a fermionic system ([3] and [4]). When atomic systems made up of bosons and fermions are considered, a very rich scenario opens up ([3], [4], [5]). In particular, Bose-Fermi mixtures sympathetically cooled into their quantum degenerate states ([6] and [7]). In the strongly interacting case, as in $^4$He systems, ([21] and [22]), supersolids have been proposed to exist and analyzed numerically in various model systems describing interacting bosons on a lattice [23].

In this paper, we consider mixtures of spinless bosons and not spin-polarized fermions, so that a non zero s-wave interaction between fermions on the same site emerges. The goal of the present work is analyzing the effects of such an interaction on phase diagrams of the system. Approaching the problem within the linear response theory framework [16, 18, 19], we show that it is possible to calculate in explicit way an effective boson-boson interaction also when the on-site fermion-fermion interaction is taken into account.

The basic idea relies on sharing tasks between the fermions and the bosons. In particular, the fermions are tuned through a density wave instability establishing crystalline order (DLRO), while the bosons provide the off-diagonal long range order (ODLRO). The interaction between bosons and fermions, and the interaction between the fermions, produce an additional density modulation also in the bosonic density field, hence resulting in a SS phase. To triggering a Density Wave (DW) instability in the fermions, the mixed boson-fermion system is confined to two dimensions and loaded in an optical lattice providing perfect Fermi surface nesting at half-filling [24]. The Supersolid transition triggered by the fermions competes with an instability towards Phase Separation in the boson system. Because of the dimensionality and the lattice geometry of our system, the presence of Van Hove singularities ([25] and [16]) -well studied
in BCS superconductivity \cite{26}, strongly enhances the
tendency towards Phase Separation and produces new
and interesting features in this transition: an arbitrary
weak interaction between the bosons and the fermions,
and between fermions, is sufficient to drive the Phase
Separation at low temperatures. In the following, we
investigate the instabilities towards Phase Separation
and Density Wave formation. We focus on the weak
coupling limit between the bosons and the fermions
and between fermions, which excludes a demixing in a
repulsive Bose-Fermi system along the lines discussed in
\cite{27}.

The organization of paper is as follows. In the section
II, we set the notation, and derive the model Hamilton-
ian. In the third section, we display the novel result
\cite{27}, where the lattice depth \(V_F\) is assumed the
same for both the spin configurations. In the experiments,
the 2D setup is realized by generating an anisotropic
three-dimensional optical potential
\(V_{B,F}(x,y) = V_B,F(\sin^2 \frac{\pi x}{a} + \sin^2 \frac{\pi y}{a}) + V_{B,F}^0 \sin^2 \frac{\pi z}{a}\)
with \(V_{B,F}^0 \gg V_{B,F}\); then the interplane hopping is
quenched.

Due to the strong localization around each lattice site \(\vec{\tau}\),
the annihilation (creation) bosonic and fermionic
field operators \(\hat{\Psi}_\alpha\) may be expanded in terms of
the Wannier functions \(w_\alpha^l(\vec{r} - \vec{\tau})\), with \(l\) the Bloch band
index \(\alpha\)

\begin{equation}
\hat{\Psi}_{\alpha}(\vec{r}) = \sum_{i,l} \hat{a}_l^\dagger w_\alpha^l(\vec{r} - \vec{\tau}_i),
\end{equation}

where \(\hat{a}_l^\dagger\) is the bosonic (\(\hat{b}_l^\dagger\)) or fermionic (\(\hat{c}_l^\dagger\,\sigma\)) annihila-
tion operator acting on a particle at the \(i\)th lattice site
and in the \(l\)th Bloch band. For a strong optical lattice
\(V_{B,F} > E_{B,F} = 2\hbar^2\pi^2/\lambda^2m_{B,F}\) the restriction
to the lowest Bloch band (\(l = 0\)) is justified \cite{1}. The translationally
invariant lattice version of Hamiltonian \(\hat{H}\) reads

\begin{equation}
\hat{H} = -J_B \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j - J_F \sum_{\langle i,j \rangle, \sigma} \hat{c}_i^\dagger,\sigma \hat{c}_j,\sigma + \frac{U_{BB}}{2} \sum_i \tilde{n}_i(\tilde{n}_i-1) + U_{BF} \sum_i \tilde{n}_i m_{i,\sigma} + U_{FF} \sum_i \tilde{m}_{i,\sigma} + \frac{\delta}{2} \sum_i (\tilde{m}_{i,\uparrow} - \tilde{m}_{i,\downarrow}) \, ,
\end{equation}

where we have omitted the band index \(l = 0\). The sym-
bol \(\langle i,j \rangle\) denotes couples of nearest-neighbor lattice
sites, and \(\delta\) the imbalance between spin-up and spin-
down fermions; \(\tilde{n}_i = \hat{b}_i^\dagger \hat{b}_i\) and \(\tilde{n}_i,\sigma = \hat{c}_i^\dagger,\sigma \hat{c}_i,\sigma\) are
the number operators for bosons and fermions with spin \(\sigma\) at
the \(i\)th site, respectively. The boson-boson, boson-fermion,
and fermion-fermion interaction amplitudes are
\(U_{BB} = g_{BB} \int d\vec{r} |w_B(\vec{r})|^4\),
\(U_{BF} = g_{BF} \int d\vec{r} |w_B(\vec{r})|^2 |w_F(\vec{r})|^2\), and
\(U_{FF} = g_{FF} \int d\vec{r} |w_F(\vec{r})|^4\), respectively \cite{1,3}.

Here, we assume a repulsive interaction between the
bosons: \(g_{BB} = 4\pi\hbar^2a_{BB}/m_B > 0\), where \(a_{BB}\) is associ-
ated the s-wave scattering length. The boson-fermion
interaction strength \(g_{BF} = 4\pi\hbar^2a_{BF}/m_B\) is assumed
to be the same for both the spin configurations; here,
\(a_{BF}\) is the boson-fermion s-wave scattering length and
\(m_B = m_Bm_F/(m_B + m_F)\) is the reduced mass. Finally,
\(g_{FF} = 2\pi\hbar^2a_{FF}/m_F\) with \(a_{FF}\) the fermion-fermion s-
wave scattering length. In the following we always as-
sume both \(a_{BF} > 0\) and \(a_{FF} > 0\).

The optical lattice with wave length \(\lambda\) provides
an \(a = \lambda/2\)-periodic potential for the bosons and
fermions with
\(V_{B,F}(x, y) = V_{B,F}(\sin^2 \frac{\pi x}{a} + \sin^2 \frac{\pi y}{a})\)
\cite{29}, where the lattice depth \(V_F\) is assumed the
same for both the spin configurations. In the experiments,
the 2D setup is realized by generating an anisotropic
three-dimensional optical potential
\(V_{B,F}(x, y) = V_{B,F}(\sin^2 \frac{\pi x}{a} + \sin^2 \frac{\pi y}{a}) + V_{B,F}^0 \sin^2 \frac{\pi z}{a}\)
with \(V_{B,F}^0 \gg V_{B,F}\); then the interplane hopping is
quenched.

Among the adavantages provided by optical lattices,
there is the possibility of tuning the Hamiltonian param-
eters in such a way to realize different interaction regimes.
Here we focus on weak coupling regime, which takes place
when \(\lambda_{BF} = U_{BF}^2N_0/U_B > < 1\) \((N_0 = 1/2\pi^2 J_F)\) and
\(t_B = 8J_B/n_BU_{BB} > > \lambda_{BF}\), where \(n_B\) is the bosonic fill-
ing factor.

The parameters involved in the Hamiltonian \(\mathcal{H}\) are re-
lated to characteristic quantities of the optical potential according to

\[ J_{B,F} = (4\sqrt{\pi})E_{B,F}^{3/4}\lambda^{3/4}\exp(-2\sqrt{V_{B,F}}); \]

\[ \frac{U_{BB}}{E_{F}^{N}} = 8\sqrt{\pi} \left( \frac{1 + m_{B}/m_{F}E_{BB}}{1 + \sqrt{V_{F}^{2}/V_{B}^{2}}} \right) \gamma \left( V_{B}^{2}/V_{F} \right)^{1/4} \gamma \left( V_{B}^{2}/V_{F} \right)^{1/2}; \]

\[ \frac{U_{BB}}{E_{F}^{N}} = 8\sqrt{\pi} \gamma \left( V_{B}^{2}/V_{F} \right)^{1/4} \gamma \left( V_{B}^{2}/V_{F} \right)^{1/2}; \]

\[ \frac{U_{FF}}{E_{F}^{N}} = 8\sqrt{\pi} \gamma \left( V_{B}^{2}/V_{F} \right)^{1/4} \gamma \left( V_{B}^{2}/V_{F} \right)^{1/2}. \]  

(4)

where \( \gamma = 2a_{z}/\lambda \). The hopping and the atom-atom interaction amplitudes \( A_{i} \) are evaluated by extending to our case the calculations performed in \[1, 3, 12\].

By exploiting the discrete Fourier transform of \( \hat{a}_{i} \) and of its Hermitian conjugate, the Hamiltonian \( \hat{H} \) may be written in the momenta space

\[
\hat{H} = \sum_{\vec{k}} \left[ \epsilon_{\sigma,\vec{k}} \hat{b}_{\vec{k}}^{\dagger} \hat{b}_{\vec{k}} + (\epsilon_{\uparrow,\vec{k}} - \delta) \hat{c}_{\uparrow,\vec{k}}^{\dagger} \hat{c}_{\downarrow,\vec{k}} + (\epsilon_{\downarrow,\vec{k}} + \delta) \hat{c}_{\downarrow,\vec{k}}^{\dagger} \hat{c}_{\uparrow,\vec{k}} \right] + \frac{1}{M^{2}} \sum_{\vec{k}} \left[ \frac{U_{BB}}{2} \hat{n}_{\vec{k}} \hat{n}_{-\vec{k}} + U_{BF} \hat{n}_{\vec{k}} \hat{m}_{-\vec{k}} + U_{FF} \hat{m}_{\vec{k}} \hat{m}_{-\vec{k}} \right],
\]

(5)

where \( M \) is the number of lattice sites in \( x \) (\( y \)) direction. We assume the wave vector \( \vec{k} \) be restricted to the first Brillouin zone: \( k_{x} \in [-\pi/a, \pi/a] \), \( k_{y} \in [-\pi/a, \pi/a] \). The density number operators are \( \hat{n}_{\vec{k}} = \sum_{\vec{p}} \hat{b}_{\vec{p}+\vec{k}}^{\dagger} \hat{b}_{\vec{p}}^{\dagger} \), \( \hat{m}_{\vec{k}} = \sum_{\vec{p}} \hat{c}_{\vec{p}+\vec{k}}^{\dagger} \hat{c}_{\vec{p}}^{\dagger} \) [19]: the bosonic and fermionic dispersion relations \( \epsilon_{\sigma,\vec{k}} \) and \( \epsilon_{\sigma,\vec{k}} \) read \( \epsilon_{\sigma,\vec{k}} = -2J_{B}(2 - \cos(k_{x}a) - \cos(k_{y}a)) \) and \( \epsilon_{\sigma,\vec{k}} = -2J_{F,\sigma}(\cos(k_{x}a) - \cos(k_{y}a)) \) [28].

III. PHASE SEPARATION VERSUS SUPERSOLID

In this section, we want to gain analytical insight into stability of the mixture ground state. As explained in [12], to achieve such a goal, the starting point is the derivation of an effective Hamiltonian for the bosons alone, by keeping in mind that fermions enters the description of our system via a modified interaction between the bosons themselves. Within linear response theory [16, 19] the boson density \( n_{B}(\vec{q}) \) (for the sake of simplicity, we refer to \( n_{B}(\vec{q})(m_{\sigma}(\vec{q})) \) as to the induced perturbation) drives the fermionic system through the following modulation of the density

\[ < m_{\sigma,\vec{q}} > = \chi_{\sigma}(U_{BF}n_{B,\vec{q}} + U_{FF} < m_{-\sigma,\vec{q}}>). \]

(6)

The function \( \chi_{\sigma} \), for the \( \sigma \) component of the spin, is the Lindhard function depending upon the absolute temperature \( T \) and on the wave vector \( \vec{q} \) [16, 19]:

\[ \chi_{\sigma}(T, \vec{q}) = \frac{1}{2} \int \frac{d\vec{k}}{v_{0}} f(\epsilon_{\sigma,\vec{k}}) - f(\epsilon_{\sigma,\vec{k}+\vec{q}}) \]

(7)

where \( v_{0} = (2\pi/a)^{2} \) is the volume of the first Brillouin zone; the integration is performed over this region. The temperature \( T \) enters via the Fermi distribution function \( f(\epsilon_{\sigma,\vec{k}}) = 1/(1 + \exp((\epsilon_{\sigma,\vec{k}} - \mu_{F})/T)) \), with \( \mu_{F} \) the chemical potential of the fermionic atoms.

We analyze the behavior of the system for temperatures well below the superfluid transition temperature \( T_{KT} \) (Kosterlitz-Thouless). Hence, the mixture is enhanced in a sufficiently low temperature regime so that the fermionic chemical potential \( \mu_{F} \) my be safely identified with the Fermi energy \( E_{F} \).

Proceeding form the Hamiltonian [13], we integrate out the fermionic freedom degrees following the same path as
Within the procedure of tracing out the fermions, we treat the spin-up component independently from the other, i.e. we perform a mean-field approximation. We get the Hamiltonian

\[ \hat{H}_{eff}^{int} = \frac{1}{M^2} \sum_{\vec{k}} \left[ \frac{U_{BB}}{2} \hat{n}_{B,\vec{k}} \hat{n}_{B,-\vec{k}} + U_{BB} (\hat{n}_{B,\vec{k}} < \hat{m}_{1,-\vec{k}} > + \hat{n}_{B,-\vec{k}} < \hat{m}_{1,-\vec{k}} >) + U_{FF} (\hat{n}_{B,\vec{k}} < \hat{m}_{1,\vec{k}} > < \hat{m}_{1,-\vec{k}} >) \right], \quad (8) \]

which describes the effective interaction between the bosons of the mixture. By employing the rules summarized in Eq. (9) in the Hamiltonian (8), we obtain

\[ \hat{H}_{eff}^{int} = \frac{1}{M^2} \sum_{\vec{k}} \left[ U_{BB} (\hat{n}_{B,\vec{k}} (\chi_1 U_{BF} \hat{n}_{B,-\vec{k}} + \chi_1 U_{FF} < \hat{m}_{1,-\vec{k}} >) + U_{BF} (\hat{n}_{B,\vec{k}} (\chi_1 U_{BF} \hat{n}_{B,-\vec{k}} + \chi_1 U_{FF} < \hat{m}_{1,-\vec{k}} >) + U_{FF} (\chi_1 U_{BF} \hat{n}_{B,\vec{k}} + \chi_1 U_{FF} < \hat{m}_{1,\vec{k}} > (\chi_1 U_{BF} \hat{n}_{B,-\vec{k}} + \chi_1 U_{FF} < \hat{m}_{1,-\vec{k}} >)) \right]. \quad (9) \]

We exploit the rules (9) in Eq. (9) in iterative way. Then, the Hamiltonian (9) can be expressed as an expansion in series of powers of \(|\chi_\alpha U_{FF}|\); we have verified that this last quantity is much smaller than one. We assume to be in a situation in which the spin-up population is equal to the spin-down one \((\delta = 0)\), and in which the fermions are in half-filling configuration, \(E_F = 0\) and \(m_\uparrow = m_\downarrow = 1/4\). In such a situation the series associated to the Hamiltonian (9) may be summed. We employ the fact that when \(\delta = 0\), is \(\epsilon_1 = \epsilon_\uparrow \equiv \epsilon_F\) and then \(\chi_1 = \chi_\downarrow \equiv \chi\), with

\[ \chi(T, \vec{q}) = \frac{1}{2} \int \frac{d\vec{k}}{v_0} f(\epsilon_{F,\vec{k}}) - f(\epsilon_{F,\vec{k}+\vec{q}}), \quad (10) \]

Together with these two last properties, we use the symmetry \(\epsilon_{F,\vec{k}} = \epsilon_{F,-\vec{k}}\); then, the effective boson-boson interaction (9) reads

\[ \hat{H}_{eff}^{int} = \frac{1}{2M^2} \sum_{\vec{k}} \left[ U_{BB} + 2\chi(T, \vec{q}) U_{BF}^2 \left( \frac{1}{1 - \chi(T, \vec{q}) U_{FF}} + \frac{U_{FF}}{(\chi(T, \vec{q}) U_{FF} - 1)^2} \right) \right] \hat{n}_{B,\vec{k}} \hat{n}_{B,-\vec{k}}. \quad (11) \]

The effective boson-boson interaction \(U_{eff}(T)\) depends on the temperature according the formula

\[ U_{eff}(T) = U_{BB} + 2\chi(T, \vec{q}) U_{BF}^2 \left( \frac{1}{1 - \chi(T, \vec{q}) U_{FF}} + \frac{\chi(T, \vec{q}) U_{FF}}{(\chi(T, \vec{q}) U_{FF} - 1)^2} \right). \quad (12) \]

The novelty of the present work relies on Eq. (12). Such a formula represents a very useful tool for investigating in analytical way the instability related to the Van Hove singularity and the one associated to the Density Wave. In particular, we are interested in calculating the temperatures of transition to PS and to DW phases. To this end, let us focus on fermionic dispersion relation \(\epsilon_{F,\vec{k}} = -2J_F [\cos(k_x a) + \cos(k_y a)]\). By analyzing \(\epsilon_{F,\vec{k}}\), we realize that the Lindhard function (10) exhibits two logarithmic singularities. These two singularities give rise to instabilities in the system. In particular, the singularity at \(\vec{q} = 0\) induces an instability towards Phase Separation. On the other hand, in correspondence of the wave vector \(\vec{k}_{DW} = (\pi/a, \pi/a)\) - which joints the saddle points (SP) \(\vec{k}_{SP} = (0, \pm \pi/a), (\pm \pi/a, 0)\) of the fermionic dispersion relation - the fermionic energy vanishes. The wave vector \(\vec{k}_{DW}\) drives a Density Wave, responsible for the Super-solid order.

Let us focus on the logarithmic Van Hove singularity, and analyze the density states. Due to the balance between the spin-up and the spin-down populations, we have that
the energy representation of the response function, in the energy representation, reads

\[ N(\epsilon) = \frac{1}{2} N_0 K \left[ 1 - \frac{\epsilon (\epsilon + \delta)^2}{16 J_F^2} \right] \approx \frac{N_0}{2} \ln \frac{16 J_F}{\epsilon (\epsilon + \delta)}, \quad (13) \]

with \( K[k] \) the complete elliptic integral of the first kind \[30\].

We write the response function \[(10)\] in the energy space \[16\], and analyze it at \( q = 0 \) and in the limit of zero temperature

\[ \chi(T \to 0, 0) = \int_0^{8 J_F} d\epsilon N(\epsilon) \delta(\epsilon) f(\epsilon)_{E_F=0} \]

\[ \sim -\frac{N_0}{2} \ln \left( \frac{16 c_1 J_F}{T} \right), \quad (14) \]

where \( 8 J_F \) is the bandwidth, and the subscripts \( \delta = 0 \)

\[ T_{PS} = 16 c_1 J_F \exp \left( \frac{2}{N_0 U_{FF} - (1 + \sqrt{1 - \frac{2 N_0 U_{FF}}{\lambda_{BF}}} \lambda_{BF})} \right) \]. \quad (16)

Let us focus, now, on the instability in the system triggered by \( \vec{k}_{DW} \). By exploiting the symmetry \( \epsilon_{F,\vec{q}} + \epsilon_{DF} = -\epsilon_{F,\vec{q}} \), the energy representation of the response function, in the energy representation, reads

\[ \chi(T, \vec{k}_{DW}) = \int_0^{8 J_F} d\epsilon N(\epsilon) \frac{\tanh(\epsilon/2T)}{-2\epsilon} \]

\[ \sim -\frac{N_0}{4} \left( \ln \left( \frac{16 c_1 J_F}{T} \right) \right)^2. \quad (17) \]

Within Bogoliubov theory, the bosonic quasiparticle spectrum is \[31\]

\[ E_B(\vec{q}) = \sqrt{\epsilon_B(\vec{q})^2 + 2n_B\epsilon_B(\vec{q})[U_{eff}(T)]}. \quad (18) \]

The induced attraction between the bosons reduces the energy of quasiparticle providing a roton minimum at \( \vec{k}_{DW} \), which vanishes at critical temperature \( T_{DW} \) given by

\[ T_{DW} = 16 c_1 J_F \exp \left[ -2 \left\{ \frac{1}{-N_0 U_{FF} + \frac{2\lambda_{BF}}{2 + t_B} + \frac{2\lambda_{BF}}{2 + t_B}} \right\} \right]. \quad (19) \]

By performing the limit \( U_{FF} \to 0 \) in Eq. \[16\] and in Eq. \[19\] we are able to reproduce the temperatures signing the Phase Separation and Density Wave calculated in \[12\].

The fermion-fermion interaction plays a crucial role in determining the order characterizing the ground state of the mixture. The interaction between the fermions influences the behavior of the system via the expression of the effective boson-boson interaction, as summarized in Eq. \[12\]. A non vanishing repulsive fermion-fermion interaction acts in such a way to rising a barrier of poten-
IV. CONCLUSIONS

In this paper, we have investigated the ground state of a Bose-Fermi mixture loaded in a two-dimensional periodic geometry, and made up of spinless bosons and not spin-polarized fermions. We have analyzed the competition between Phase Separation and Supersolid orders. This analysis was carried out within the framework of the linear response theory. By employing an iterative technique, we have obtained an analytical expression for the effective boson-boson interaction as a function of the absolute temperature of the sample. We have performed our study in absence of fermionic population imbalances and in presence of boson-fermion and fermion-fermion repulsive interactions. We have studied the phase diagram of the system by stressing the role of the fermion-fermion interaction in determining the kind of order sustained by the Bose-Fermi mixture.
Hamiltonian. We have explained the changes that such an interaction introduces in the behavior of the system with respect to the case in which the fermions do not interact on the same lattice site. We have discussed the nice interplay between the critical value of the optical lattice depth for the fermions and the temperature of the sample in establishing the kind of order in the ground state of the mixture.

The study of such a topic opens up a bunch of very exciting possibilities. In particular, a very interesting relationship could be established between these issues and the ones related to propagation of the zero sound waves both in homogeneous [18] and in trapped [32] systems of ultracold atoms; for these kind of problems, in fact, the linear response theory is exploited as well.

In a forthcoming paper, we wish to accomplish the task of analyzing the case of imbalance between the two fermionic populations and different sign of boson-fermion and fermion-fermion interactions, by employing a suitable modification of the iterative method displayed in the present work.

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