Abstract

A mixture of spin-1/2 fermionic atoms and molecules of paired fermionic atoms is studied in an optical lattice. The molecules are formed by an attractive nearest-neighbor interaction. A functional integral is constructed for this many-body system and analyzed in terms of a mean-field approximation and Gaussian fluctuations. This provides a phase diagram with the two merging Mott insulators and an intermediate superfluid. The Gaussian fluctuations give rise to an induced repulsive dimer-dimer interaction mediated by the unpaired fermions. The effect of an unbalanced distribution of spin-up and spin-down fermions is also discussed.

1 Introduction

A wide new field for investigating complex many-body systems has been opened by the idea that clouds of atoms can be cooled to very low temperatures by sophisticated cooling techniques [1]. Such an atomic cloud can be brought into a periodic potential which is created by counterpropagating laser fields [2]. This potential mimics the lattice of core atoms of a solid-state system and is called optical lattice due to its origin. It allows the simulation of conventional condensed-matter systems as well as the creation of new many-body systems. New quantum states can emerge due to the interplay of tunneling and interaction between the atoms.

In the following, a cloud of spin-1/2 fermionic atoms in an optical lattice is considered, where an attractive interaction between atoms in nearest-neighbor lattice wells is assumed. Our aim is to study different quantum phases that can appear due to the formation and dissociation of molecules, and condensation of the (bosonic) molecules.

2 Model

Our atomic cloud in an optical lattice is described by a grand-canonical system of spin-1/2 fermions at temperature $1/\beta$ and chemical potentials $\mu_1$ and $\mu_2$, referring to the two possible projections of the spin. Its partition function is defined as a functional integral with respect to Grassmann fields as [3] [4]:

$$Z = \int e^{S(\psi, \bar{\psi})} D[\psi, \bar{\psi}],$$

(1)
where $S$ is the action

$$S(\psi, \bar{\psi}) = \int_0^\beta \left[ \sum_r \left( \psi^1_r \partial_\tau \bar{\psi}^1_r + \psi^2_r \partial_\tau \bar{\psi}^2_r \right) - \sum_r \left( \mu_1 \psi^1_r \bar{\psi}^1_r + \mu_2 \psi^2_r \bar{\psi}^2_r \right) \right] d\tau - \frac{t}{2d} \sum_{\langle r,r' \rangle} \left( \psi^1_r \bar{\psi}^1_{r'} + \psi^2_r \bar{\psi}^2_{r'} \right) - \frac{J}{2d} \sum_{\langle r,r' \rangle} \psi^1_r \bar{\psi}^1_{r'} \psi^2_r \bar{\psi}^2_{r'} d\tau.$$ \hspace{1cm} (2)

t is the tunneling rate of single fermions, whereas $J$ is the rate for tunneling of a pair of fermions, located at nearest-neighbor sites in the optical lattice. The $J$-term represents an attractive interaction. In contrast to a local interaction, it provides a dynamics for the molecules. Depending on the ratio $t/J$, there is a competition between the individual fermion dynamics (dominating for $t/J \gg 1$) and the dynamics of molecules (dominating for $t/J \ll 1$).

### 3 Mean-field approximation and Gaussian fluctuations

We decouple the $J$-term in the functional integral by two complex fields $\phi$ and $\chi$ \[3,4\]. $\phi$ is related to the order parameter for the formation of molecules, and $\chi$ is required for stabilizing the complex integral. A subsequent integration over the Grassmann fields leads to

$$S_{\text{eff}} = \int_0^\beta \left\{ \sum_{r,r'} \bar{\phi}_r \partial_\tau \bar{\phi}_{r'} + \frac{1}{2J} \sum_r \bar{\chi}_r \chi_r - \ln \det \hat{G}^{-1} \right\} d\tau,$$ \hspace{1cm} (3)

where

$$\hat{G}^{-1} = \begin{pmatrix} -i\phi - \chi & \partial_\tau + \mu_1 + t\hat{w} \\ \partial_\tau - \mu_2 - t\hat{w} & i\phi + \bar{\chi} \end{pmatrix},$$

and a nearest-neighbor matrix $\hat{w}$ whose elements are $1/2d$ on the $d$-dimensional lattice. Moreover, we have $\hat{v} = J(\hat{w} + 2\hat{1})$. The saddle-point (SP) approximation $\delta S_{\text{eff}} = 0$ for uniform fields and $\mu_1 = \mu_2$ leads to the BCS-type mean-field result:

$$\chi = -\frac{2i\phi}{3}, \quad \frac{1}{J} = G,$$ \hspace{1cm} (4)

with

$$G = \frac{1}{\beta} \sum_{\omega_n} \int_{-1}^1 \frac{\rho(x)}{|\phi|^2/9 - (i\omega_n + \mu_1 + tx)(i\omega_n - \mu_2 - tx)} dx,$$ \hspace{1cm} (5)

and the density of states $\rho$ of free particles in the optical lattice. The mean-field calculations gives three phases: an empty phase, a Mott insulator and a Bose-Einstein condensate (BEC) of the molecules whose condensate density is

$$n_0 = \frac{|\phi|^2}{9J^2}.$$ \hspace{1cm} (6)

The latter is plotted in Fig. 1 and the phase diagram is shown in Fig. 2.

Excitations out of the molecular BEC can be described by Gaussian fluctuations around the SP solution by complex fields $\phi$ and $\chi$. Using $\Delta = i\phi + \chi$, $\widetilde{\Delta} = i\phi + \bar{\chi}$, the corresponding action is

$$S_{\text{eff}} = S_{\text{eff}}^0 + \delta S_{\text{eff}}$$ \hspace{1cm} (7)
with
\[
\delta S_{\text{eff}} = \int_0^\beta \left\{ \sum_{r,r'} \delta \tilde{\phi}_r \dot{\tilde{\phi}}_{r'}^{-1} \delta \phi_{r'} + \frac{1}{2J} \sum_r \delta \tilde{\chi}_r \delta \chi_r \right\} d\tau - \frac{1}{2\beta} \text{tr} \left[ \hat{G}_0 \left( \begin{array}{cc} -\delta \Delta & 0 \\ 0 & \delta \Delta \end{array} \right) \right]^2. \tag{8}
\]

The above result reads in terms of Fourier coordinates
\[
\delta S_{\text{eff}} = \sum_{q,\omega} \langle \delta \tilde{\phi}_{q,\omega}, \hat{G}_{\text{eff}}^{-1}(q, i\omega) \delta \phi_{q,\omega} \rangle, \tag{9}
\]
where \( \hat{G}_{\text{eff}}^{-1} \) is a 4 by 4 propagator, \( \delta \phi \) is a four-component spinor. More details of the calculation can be found in Ref. [4]. The excitation spectrum \( \epsilon_q \equiv i\omega(q) \) is the solution of
\[
det \hat{G}_{\text{eff}}^{-1}(q, i\omega) = 0. \tag{10}
\]

This gives the Bogoliubov spectrum in the molecular BEC and a gapped spectrum outside the BEC (see Fig. 3).

### 4 Discussion and Conclusions

Our mean-field approach also allows us to consider an unbalanced molecular condensate [5, 6] by imposing different chemical potentials for the two spin projections of the fermions, \( \mu_1 = \mu + h, \mu_2 = \mu - h \). Although we cannot address questions about nonlocal properties (like phase separation [7, 8, 9]) directly within our mean-field approach, the effect of two chemical potentials provides interesting effects even in a uniform system. In particular, the existence of a first-order phase transition, usually leading to phase separation, can be studied with the mean-field action of the unbalanced system
\[
S_{\text{eff}} \sim \frac{\left| \phi \right|^2}{9J} - \frac{1}{\beta} \int_1 \rho(x) \ln \left[ \cosh \left( \frac{E_+(x)\beta}{2} \right) \cosh \left( \frac{E_-(x)\beta}{2} \right) \right] dx, \tag{11}
\]
where
\[
E_\pm(x) = -h \pm \sqrt{\left| \phi \right|^2/9 + (\mu + tx)^2}. \tag{12}
\]

This gives a first order-phase transition due to two separated minima in the mean-field action for small \( \mu \) or for larger \( \mu \), depending on \( h \) and \( t \) (for fixed \( J \)) (cf. Fig. 4).

For small single-fermion tunneling rate \( t \), there is a spin-polarized phase simply because one spin projection has a negative chemical potential. This can happen for small \( \mu \) (cf. Fig. 5). If \( t \) is larger, there is a shift of the chemical potential in Eq. (12) by the single-fermion tunneling rate. This prevents the appearence of a spin-polarized state for small \( \mu \) but it leads to a sudden disappearence of the molecular condensate at large \( |\mu| \), as shown in Fig. 5. This is accompanied by a first-order phase transition. At the point \( h = \mu \) there might be a coexistence of molecules and spin polarized fermions [10, 11].

In conclusion, our mean-field approach to the model of Eq. (2) reduces to a BSC-type theory of molecules for spin-1/2 fermions with attractive interaction. It also provides a Mott insulator and a spin-polarized phase. The Gaussian fluctuations describe Bogoliubov-type excitations of a molecular condensate and the gapped excitation spectrum of a Mott insulator.
Figure 1: Density of a molecular condensate for different single-fermion tunneling rates $t$. $\mu$ and $t$ are in units of $J$.

Figure 2: Phase diagram for different values of $t$. 

BEC

Mott insulator, $n=1$

Empty phase, $n=0$
Figure 3: Quasiparticle excitations for $t = 0.5$ and $J = 1$.

Figure 4: Mean-field action of an unbalanced system, indicating a first-order transition from the molecular condensate with increasing $h = (\mu_1 - \mu_2)/2$. For $t = 0.2, \mu = 0$ and zero temperature the transition takes place around $h = 0.25$. 
Figure 5: Density of a molecular condensate as a function of \((\mu_1 + \mu_2)/2\) for \(h = 0.26, J = 1, T = 0\).

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