acta physica slovaca vol. 49 No. 4, 605 – 612 August 1999

PAIRING OF FERMIONS IN OPTICAL LATTICES*

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Received 5 May 1999, accepted 10 May 1999

We consider weakly interacting fermionic atoms in optical lattices. We show that the system can be described by the Hubbard model, and solve the BCS gap equations. Cooper-pairing is shown to take place for parameter values which are obtainable for alkali atoms in optical lattices.

PACS: 05.30.Fk, 32.80.Lg, 71.10.Fd, 74.20.Fg

1 Introduction

Advances in the theory and experiments of trapping and cooling atoms with laser light [1] have lead to achievements of remarkable significance. For example, the successes in producing Bose-Einstein condensates of trapped alkali atoms [2] have made it possible to experimentally test various fundamental effects of quantum statistics. In addition to enlightening us on fundamentals, atomic condensates may be the road to develop the atom laser [3]. Other applications of Bose-condensates could be found e.g. in quantum computing [4].

Trapping and cooling of *fermionic* isotopes of alkali atoms by means of symphatetic cooling is in progress. In the experiments on trapping ^{6}Li in 1995 the temperatures reached were of the order of milli-Kelvin [5], and in 1998 temperatures of $T \sim 50\mu K$ we obtained for ^{40}K [6]. Very recently successful cooling of ^{40}K atoms down to $T \sim 0.5\mu K$ was reported (see [7]). This temperature is already of the same order of magnitude as the Fermi-temperature, thus degenerate Fermi gases are expected to be available in the near future. This has begun to inspire theoretical studies as well [8–11].

Weakly interacting degenerate atomic Fermi gases would allow to realize and test many models used in solid state physics, such as the BCS-theory of electron pairing, the advantage being that the atomic counterparts of solid state systems are generally much cleaner and the system parameters are easily controllable (usually due to the high controllability of laser light). Open questions related to topics of paramount fundamental and technological importance, such as high-T_c superconductivity, are expected to aquire illumination through the studies of cold

*Presented at the 6th Central-European Workshop on Quantum Optics, Château Chudobín, Czech Republic, April 30 - May 3, 1999.

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fermionic atoms. Moreover, atoms have more internal degrees of freedom than electrons, and are easily manipulated by laser light, thus completely novel quantum many-body effects may be found. Another speciality of the atomic systems is the variety of confining geometries that can be produced by different kinds of optical and magnetic traps and lattices.

In this paper we consider weakly interacting fermionic atoms in an optical lattice, and ask the question whether BCS-type pairing takes place in such a system. We first show that the Hubbard model [12] can be used to describe fermions in an optical lattice. In the simplest case, the model parameters all depend on the properties of the optical lattice potential in such a way that they cannot be tuned independently [13]. We show, however, that with parameter values which are actually obtainable, Cooper-pairing takes place. This implies that optical lattices can be used to test and develop BCS-type theories of many-body quantum effects, and to search for answers to related open questions. One such question is the cross-over from the BCS ground state for weakly interacting particles to Bose-condensation of bound pairs in the limit of strong interactions. The cross-over transition is claimed to be smooth [15–17], yet the behaviour of the system for intermediate interaction strengths is not fully understood. Critical temperatures in the intermediate region are higher than in the BCS and BEC limits; knowledge about the ground state would contribute towards understanding high-T_c superconductivity.

In Section 2 we define the Hamiltonian of the system and transform it into the Hubbard Hamiltonian. The model parameters that can be reached in the considered system are estimated in Section 3. In Section 4 we present the results from solving BCS gap equations with these parameters. A short summary is given in Section 5.

2 Hubbard model for fermions in optical lattices

We consider fermionic atoms of mass m confined in a 2-D optical lattice potential $V^L(\mathbf{x}) = V_x \sin^2(2\pi x/\lambda) + V_y \sin^2(2\pi y/\lambda)$, where λ is the wavelength of the laser and $V_{x/y}$ are proportional to the dynamic atomic polarizability times the laser intensity. We include also the possibility of an additional external potential $V^E_\sigma(\mathbf{x})$, such as a trap or a superlattice, varying in a larger scale than the lattice. The atoms are assumed to interact via a δ-type potential characterized by a scattering length a_s. Moreover, they are regarded as two-level systems with internal degrees of freedom denoted by $\sigma = \{\uparrow, \downarrow\}$. Because the atoms are fermions, s-wave scattering is suppressed for particles of same "spin" (internal state), thus we consider only the interaction between particles with different spins. We assume the interaction to be attractive. The lattice potential is taken to be the same for both spins, whereas in the external potential we have kept the index σ. The second quantized Hamiltonian for the system is written with the help of anticommuting fermionic field operators $\psi^\dagger_\sigma(\mathbf{x})$ as (c.f. [10, 18])

$$
\begin{aligned}
\hat{H} &= \sum_\sigma \int d^2x \psi^\dagger_\sigma(\mathbf{x}) \left(-\frac{\hbar^2}{2m}\nabla^2 + V^L(\mathbf{x}) + V^E_\sigma(\mathbf{x}) \right) \psi_\sigma(\mathbf{x}) \\
&\quad + \frac{1}{2}\frac{4\pi a_s \hbar^2}{m} \int d^2x \psi^\dagger_\uparrow(\mathbf{x}) \psi^\dagger_\downarrow(\mathbf{x}) \psi_\downarrow(\mathbf{x}) \psi_\uparrow(\mathbf{x}). \qquad (1)
\end{aligned}
$$

This can be transformed into the well-known Hubbard Hamiltonian by expanding the field operators in terms of Wannier functions $w(\mathbf{x} - \mathbf{x}_j)$ [19] and of on-site fermionic annihilation operators $c_{j\sigma}$ (the index j refers to the jth site in the lattice):

$$\psi_\sigma(\mathbf{x}) = \sum_j c_{j\sigma} w(\mathbf{x} - \mathbf{x}_j). \tag{2}$$

Here and in the following $\sum_j$ denotes a summation over $j = (j_x, j_y)$ from $j = (1,1)$ to $j = (N,N)$, where N is the number of lattice sites in one dimension. The Hamiltonian becomes (c.f. the derivation in the case of bosons in optical lattice in [14])

$$\hat{H} = -J \sum_{<i,j>,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{j,\sigma} c^\dagger_{j\sigma} c_{j\sigma} V^E_{j\sigma} + U \sum_j c^\dagger_{j\uparrow} c^\dagger_{j\downarrow} c_{j\downarrow} c_{j\uparrow},$$

where $< i,j >$ denotes summation over nearest neighbours and

$$J = -\int d^2x w^*(\mathbf{x}-\mathbf{x}_i)[-\frac{\hbar^2}{2m}\nabla^2 + V^L(\mathbf{x})]w(\mathbf{x}-\mathbf{x}_j) \tag{3}$$

$$U = \frac{4\pi a_s \hbar^2}{m} \int d^2x |w(\mathbf{x})|^4 \tag{4}$$

$$V^E_{j\sigma} = \int d^2x V^E_\sigma(\mathbf{x}) |w(\mathbf{x}-\mathbf{x}_j)|^2. \tag{5}$$

For weakly interacting atoms in a lattice, momentum space description is more adequate than the real space one. By introducing the lattice momentum creation operators by $c^\dagger_{k\sigma} = \frac{1}{N}\sum_j e^{-ik\cdot j} c^\dagger_{j\sigma}$ the Hamiltonian is turned into

$$\begin{aligned} H = & -2J \sum_k (\cos(k_x) + \cos(k_y))[c^\dagger_{k\uparrow} c_{k\uparrow} + c^\dagger_{k\downarrow} c_{k\downarrow}] \\ & + \sum_{k,l,\sigma} c^\dagger_{k\sigma} c_{k\sigma} \frac{1}{N^2} \sum_j e^{i(k-l)\cdot j} V^E_{j\sigma} \\ & + \frac{U}{N^2} \sum_{k,l,q} c^\dagger_{k\uparrow} c^\dagger_{l\downarrow} c_{k-q\downarrow} c_{l+q\uparrow} \end{aligned} \tag{6}$$

The momentum $k = (k_x, k_y) = (2\pi n_x/N, 2\pi n_y/N)$, where the integers (n_x, n_y) range from $(-(N-1)/2, -(N-1)/2)$ to $((N-1)/2, (N-1)/2)$.

3 Obtainable parameters

As seen from the definitions (3)–(4) for J and U, these parameters both depend on the Wannier functions which are essentially defined by the optical lattice potential. Therefore J and U are not independently tunable by the laser parameters. There is actually a trade-off: high laser intensity, that is tight confinement in one lattice site, enhances interaction strength because the probability for the particles to overlap is large — on the other hand hopping from site to site becomes more difficult leading to small J. And reveresed, for small intensity hopping is easy but U decreases.

Following the treatment in [14], we have made an order of magnitude estimate for the obtainable parameters in the present case. Ingredients to do this estimate are, first of all, the typical scattering lengths of fermionic atoms. For ^{86}Rb and ^{22}Na the order of magnitude is $a_s \sim -100 a_B$ (a_B is the Bohr radius) [9] whereas for instance ^{6}Li has an unusually large scattering length of $a_s \sim -1000 a_B$ [8]. The hopping amplitude J is basically limited by the requirement that hopping should not take a time that is too long considering the experimental possibilities. The relevant time t and J are fixed by the requirement $Jt/\hbar \sim 1$. Setting for instance $t < 1\mu s$ restricts J from below to $J/E_R > 0.02$ (the recoil energy E_R provides a convenient scaling, we have used here $E_R = \hbar 2\pi \times 8.9kHz$ given in [14] for sodium and for $\lambda = 985nm$). According to [14], this limits $(|U|/E_R)(a/a_s) < 20$, where $a = \lambda/2$. For the scattering lengths given above, a/a_s is of the order 1 – 10, thus largest possible U/J ratio is of the order of 100 – 1000. The interaction strengths that lead to Cooper-pairing, namely $|U|/J \sim 1$, are very well below this upper limit. From below $|U|/J$ is limited by the fact that for very large J the model is no longer valid (next-nearest neighbour hopping becomes important). However, $|U|/J \sim 1$ is still well in reach.

In the numerical calculations in this paper we have chosen to use $J = 1$ and $U = \{-0.1, -2.5, -3.5\}$.

4 BCS ground state

The ground state of the Hamiltonian is searched for by using the well known BCS-ansatz

$$|\psi\rangle = \prod_k (u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow})|0\rangle, \tag{7}$$

where $u_k^2 + v_k^2 = 1$ (u_k and v_k are assumed to be real). In case of non-interacting particles, all $v_k = 1$ up to the Fermi-level. Interactions, however, introduce pairing fluctuations and u_k and v_k near the Fermi-level start to deviate from zero and one. Our goal is to see whether this happens for parameters that are obtainable in optical lattices.

The coefficients u_k and v_k which define the ground state are found by minimizing the expectation value of energy

$$\langle\psi|\hat{H}|\psi\rangle - \mu\langle\psi|\hat{N}_p|\psi\rangle. \tag{8}$$

Since the BCS-ansatz is not number-conserving, the term $-\mu\hat{N}_p$, where μ is the chemical potential, is added to the Hamiltonian in order to fix the particle number. The minimization of (8) leads to the following gap equations [20]:

$$\Delta = -\frac{4U}{N^2}\sum_{k>0} v_k\sqrt{1-v_k^2}, \tag{9}$$

$$v_k^2 = \frac{1}{2}\left[1 - \frac{\tilde{\epsilon}_k}{\sqrt{\tilde{\epsilon}_k^2 + \Delta^2}}\right], \tag{10}$$

$$\tilde{\epsilon}_k = -2J(\cos(k_x) + \cos(k_y)) + \frac{4U}{N^2}N_p - \mu, \tag{11}$$

$$N_p = 2\sum_{k>0} v_k^2. \tag{12}$$

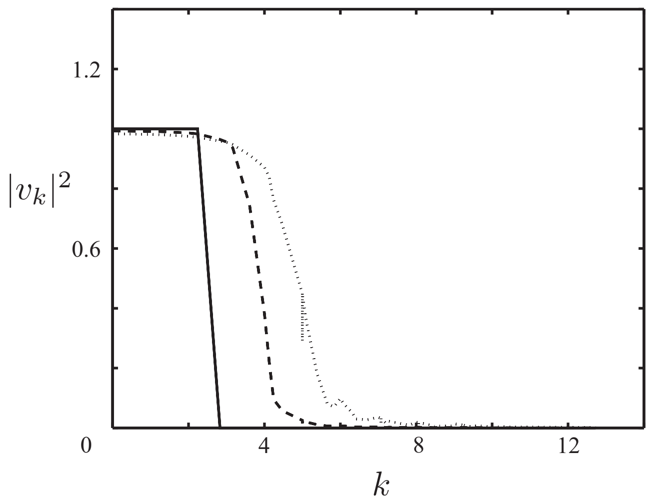

Fig. 1. The coefficient v_k^2 as a function of the absolute value of the momentum k, for three different interaction strengths U. The chemical potential $\mu = -3.5$, corresponding to the particle numbers $N_p = 16$, $N_p = 32$ and $N_p = 48$ for $U = -0.1$ (solid line), $U = -2.5$ (dashed line) and $U = -3.0$ (dotted line), respectively. The size of the lattice in this and the following figures is 21×21, that is $N = 21$.

Here N_p is the number of particles. These coupled non-linear equations have to be solved numerically. We use the parameter values $J = 1$, $\mu = -3.5$, lattice size 21×21 ($N = 21$), and three different values for the interaction strength, $U = -0.1$, $U = -2.5$ and $U = -3.0$. The external potential V^E is set to zero. Figure 1 shows that for $U = -0.1$ the distribution of v_k^2's as a function of the absolute value of k is more or less a step function, i.e. the ground state is the trivial completely filled Fermi sea. Instead for $U = -2.5$ and $U = -3.0$ pairing is indeed visible as the distribution v_k^2 starts to deviate from a step function. This is clearly seen also in Figs. 2-4, where we show 2-D plots of $v^2(k_x, k_y)$. The slightly non-smooth behaviour of the curves in Fig. 1 is due to the the projection from 2-D to 1-D in a discrete and finite lattice.

5 Discussion

We have described attractively interacting atoms in optical lattices by the Hubbard model, and shown that Cooper pairing takes place for model parameter values which are experimentally within reach. This means that BCS-theory and related open questions such as the cross-over from Cooper-pairing to Bose condensation of bound pairs can be investigated in the context of atoms in optical lattices. Atoms confined by light offer a clean and highly controllable environment for experiments, in contrast to solid state systems which are often burdened by impurities and not as easily manipulated.

The possibility to manipulate the internal degrees of freedom of the atoms by laser light opens up interesting possibilities in pairing phenomena; laser manipulation would be a way to create composite objects in a controlled manner. Laser-assisted pairing of cold fermions will be discussed in a future publication.

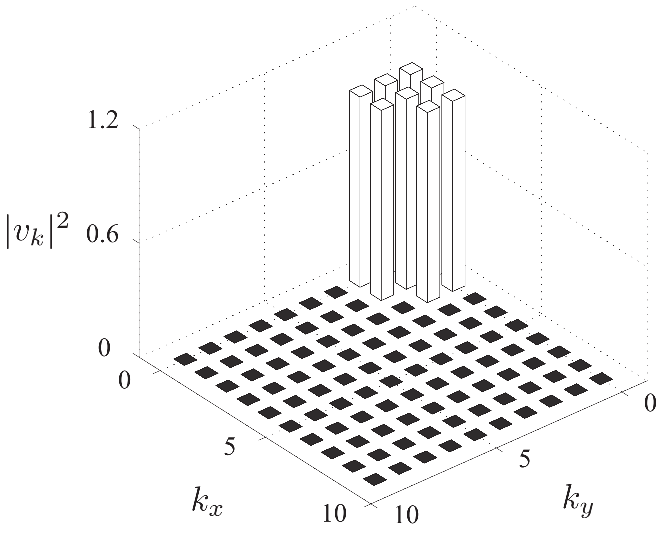

Fig. 2. The coefficient v_k^2 as a function of k_x and k_y for the interaction strength $U = -0.1$. The chemical potential $\mu = -3.5$, corresponding to the particle number $N_p = 16$. In this and the following figures $k_{x/y}$ are scaled by $2\pi/N$ ($N = 21$), and only one quarter of the k-space is shown, namely $k_x, k_y \geq 0$.

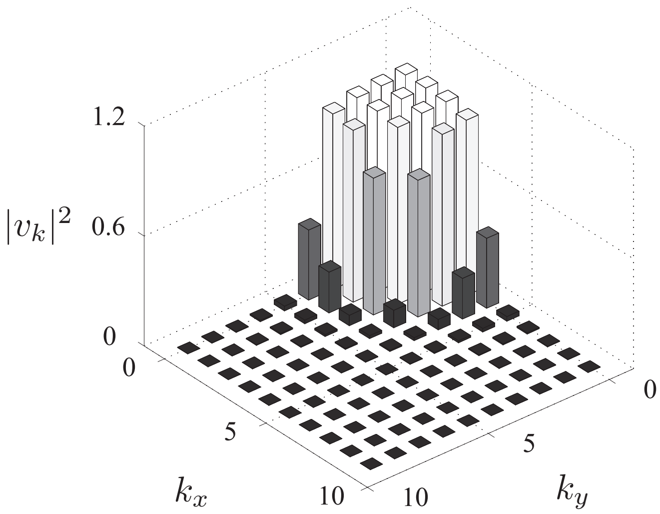

Fig. 3. The coefficient v_k^2 as a function of k_x and k_y for the interaction strength $U = -2.5$. The chemical potential $\mu = -3.5$, corresponding to the particle number $N_p = 32$.

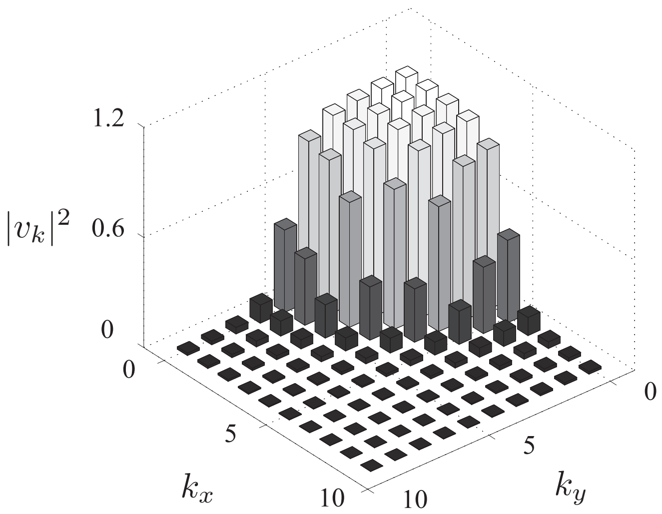

Fig. 4. The coefficient v_k^2 as a function of k_x and k_y for the interaction strength $U = -3.0$. The chemical potential $\mu = -3.5$, corresponding to the particle number $N_p = 48$.

Acknowledgments This work was supported in part by the Österreichischer Fonds zur Förderung der wissenschaftlichen Forschung, the European Community under the TMR network ERB-FMRX-CT96-0087 and the Institute for Quantum Information GmbH. P.T. acknowledges the support by the TMR Programme of the European Commision (ERBFMBICT983061) and by the Academy of Finland.

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