Interband physics in an ultra-cold Fermi gas in an optical lattice

J.-P. Martikainen,1, 2 E. Lundh,3 and T. Paananen2

1Nordita, 106 91 Stockholm, Sweden
2Department of Physics, University of Helsinki, PO Box 64, 00014 University of Helsinki, Finland
3Department of Physics, Umeå University, SE-90187, Umeå, Sweden

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We study a gas of strongly polarized cold fermions in an optical lattice when the excited \( p \)-bands are populated. We derive the relevant Hamiltonian and discuss the expected phase diagram for both repulsive and attractive interactions. In the parameter regime covered here, checkerboard anti-ferromagnetic ordering is found to be possible for repulsive interactions while for attractive interactions, transitions between different types of paired phases are predicted.

I. INTRODUCTION

Experiments with ultra-cold Fermi gases in optical lattices have opened a way to study experimentally interacting fermionic systems in a highly tunable environment [1, 2]. Among other things, in such a system one can expect a multitude of correlated fermionic phases as well as superfluidity. In a two-component fermionic gas the atom numbers of different components can be independently controlled and such strongly interacting polarized fermion gases have been recently studied experimentally [3, 4, 5]. Such studies have revealed, for example, intriguing phase separation properties and, depending on parameters, appearance of trap physics beyond the local-density approximation [6].

In this article we address the issue of a strongly polarized two-component Fermi gas in an optical lattice. Polarized Fermi gases on the lowest band have been studied previously, see for example Ref. [7], but here we wish to investigate the relevant theory as well as phases associated with it, when the majority component fills the lowest band and also populates excited bands. To this end, we derive the Hamiltonian for this system and apply it to discuss the possible phases both for repulsive as well as attractive interactions.

Multiband physics has a long history in the condensed matter theory and superconductors with several bands have been addressed within the BCS as well as Ginzburg-Landau formalism [8, 9]. However, a system of polarized ultracold atoms in optical lattices is different in many important respects. First, in the theory of transition metals, for example, the multiband description is motivated by the fact that the Fermi surface might pass through two (or more) bands. Under such circumstances there are processes which transfer electrons between bands as well as interactions inside the bands. In the system that we consider the bands are well separated and there are no processes that transfer atoms between bands. Here the interaction between the bands is proportional to the product of the densities in different bands and does not involve transfer of atoms between bands [8]. Second, in the present system only interband interactions are relevant. This makes it much easier to study interband effects without being disturbed by large inband effects. Third, the anisotropic nature of the \( p \)-band tunneling as well as the multi-flavor character of the \( p \)-band fermions gives rise to qualitatively novel possibilities. Fourth, the Hamiltonian for the system we discuss can be derived from the microscopic theory in a controlled way.

Higher band physics with Bose-Einstein condensates was experimentally studied by Müller et al. [10] and interaction induced transitions to higher bands were observed by Köhl et al. [1] while Diener and T.-L. Ho [11] tackled this problem theoretically. In this paper, however, the interaction strengths are much smaller than the bandgaps and such interaction induced higher band effects do not play an important role. Other interesting possibilities also exist. For example, the higher band atoms might have stronger nearest neighbor interactions which might make super solid phases appear in some parts of the phase diagram [12]. On the other hand when the lattice geometry is varied, unconventionally ordered quantum phases are predicted to be possible [13, 14]. Some aspects of the higher band physics in one dimension were also discussed by Kautian et al. [15] in the context of lattice excitons, by Kärkkäinen et al. [16] for repulsive interactions with high filling fractions, and by A. F. Ho [17], who focused on the equal mixture Fermi gas with strong interactions and with two atoms per site. More recently anti-ferromagnetic properties of \( p \)-band fermions at half filling were studied by Wu and Zhai [18] and \( p \)-band fermions in a two-dimensional lattice with different lattice geometries by Zhao and Liu [19].

II. HAMILTONIAN

Atoms in a cubic optical lattice experience a potential \( V_\sigma(r) = \sum_\alpha V_{\alpha,\sigma} \sin^2 \pi r_\alpha/d \), where \( \alpha = \{x, y, z\} \), \( V_{\alpha,\sigma} \) are the lattice depths for atoms of type \( \sigma \), and \( d \) is the lattice constant. Our interest is in a strongly polarized two-component gas where the majority component fills the lowest band and occupies also part of the first excited bands. We label the components by \( \uparrow \) and \( \downarrow \). A
Hubbard-model Hamiltonian for the fermions is arrived at by expanding the field operators $\psi_\alpha(r)$ in terms of the localized Wannier functions [20]. The Wannier wavefunctions on the lowest band, $w_{0,\sigma}(r)$, are even functions, while the Wannier function $w_{a,\sigma}(r)$ on the $p$-band has a node in the plane normal to the coordinate axis $\alpha$, giving rise to three types of state for the spin-up fermions which we label $x$, $y$, and $z$, respectively [21]. Including only the leading nearest neighbor tunneling terms, we find the Hamiltonian for the ideal two-component Fermi gas in momentum space

$$H_{\text{ideal}} = \sum_{\sigma, \mathbf{k}} (\epsilon_{0,\mathbf{k},\sigma} - \mu_\sigma) \psi_{0,\mathbf{k},\sigma}^\dagger \psi_{0,\mathbf{k},\sigma} + \sum_{\alpha, \mathbf{k}} (\epsilon_{\alpha,\mathbf{k},\uparrow} - \mu_\uparrow) \psi_{\alpha,\mathbf{k},\uparrow}^\dagger \psi_{\alpha,\mathbf{k},\uparrow},$$

where $\sigma = \{\uparrow, \downarrow\}$. Here the summation is over the first Brillouin zone, $\psi_{0,\mathbf{k},\sigma}^\dagger$ creates an atom in the lowest band, $\mu_\sigma$ are the chemical potentials [22], and $\epsilon_{0,\mathbf{k},\sigma}$ and $\epsilon_{\alpha,\mathbf{k},\sigma}$ are the dispersions on the lowest and excited $p$-bands respectively. Furthermore, $\psi_{\alpha,\mathbf{k},\uparrow}^\dagger$ creates a spin-up atom with momentum $\mathbf{k}$.

The lowest band dispersion is given by the usual expression $\epsilon_{0,\mathbf{k},\sigma} = \sum_{\beta=x,y,z} J_0^{\alpha,\beta} (1 - \cos(k_\beta d))$, where in principle the tunneling strength can depend on the spin-state as well as on direction if the lattice depth is different in different directions. The excited band dispersions are more complex. First, of all, the excited bands are separated from the lowest band by energy gaps $\Delta_{\alpha,\text{BG}}$. Second, since the Wannier functions on the excited band have a node and are antisymmetric along some axis, the tunneling strength for moving an atom in the direction orthogonal to the nodal plane is different from moving it in the direction along the nodal plane. The dispersions are then $\epsilon_{\alpha,\mathbf{k},\downarrow} = \Delta_{\alpha,\text{BG}} + \sum_{\beta=x,y,z} 2J_{\alpha,\beta} (1 - \cos(k_\beta d))$, where $J_{\alpha,\beta}$ is the tunneling strength in the direction $\beta$ for an atom which has a localized wavefunction $w_{\alpha}(r)$.

In ultracold gases the dominant interaction between unlike fermions is typically the $s$-wave interaction $g \int dr n_\downarrow(r)n_\uparrow(r)$, where the coupling $g$ can be expressed in terms of the $s$-wave scattering length $a$ and atomic mass $m$ as $g = 4\pi\hbar^2a/m$. This interaction term can again be reduced into the lattice by expanding the field operators and keeping only the leading on-site interaction terms. This procedure gives us a contribution in coordinate space

$$H_I = U_0 \sum_{i=(x_i,y_i,z_i)} \psi_{0,\mathbf{i},\uparrow}^\dagger \psi_{0,\mathbf{i},\uparrow} \psi_{0,\mathbf{i},\downarrow}^\dagger \psi_{0,\mathbf{i},\downarrow} + \sum_{i=(x_i,y_i,z_i)} \sum_{\alpha=(x,y,z)} U_{1,\alpha} \psi_{\alpha,\mathbf{i},\uparrow}^\dagger \psi_{\alpha,\mathbf{i},\uparrow} \psi_{0,\mathbf{i},\downarrow}^\dagger \psi_{0,\mathbf{i},\downarrow}$$

to the Hamiltonian. The coupling strength $U_0$ between atoms on the lowest band is related to the scattering length through $U_0 = g \int d^3r |w_{0,\downarrow}(r)|^2 |w_{0,\uparrow}(r)|^2$ while the interband couplings between the ↓-atoms on the lowest band and the ↑-atoms on the excited band are given by $U_{1,\alpha} = g \int d^3r |w_{0,\downarrow}(r)|^2 |w_{\alpha,\uparrow}(r)|^2$.

In principle, the localized Wannier functions could be calculated numerically from the three-dimensional band structure, but this is unnecessary for our purposes. One gets reasonable analytical estimates for all the parameters of the theory by approximating the Wannier functions with harmonic oscillator states localized at each lattice site. General features are not sensitive to precise numerical values of the parameters and the harmonic approximation gives us a handle on how various parameters vary relative to one another as the lattice depth is changed. The analytical formulas for the parameters are long and not very informative and are, for that reason, omitted here. It is however necessary to discuss some general features.

Firstly, for typical parameters the bandgaps are much higher than other energy scales of the problem. Second, in the harmonic approximation the interband coupling is simply $U_{1,\alpha} = U_0/2$ and is independent of which excited band is involved, even for an-isotropic lattices. Third, on the excited bands the diagonal tunneling strengths $J_{\alpha,\alpha}$ have an opposite sign to the off-diagonal strengths (as well as tunneling strengths on the lowest band) and also their magnitude is much larger than those for the off-diagonal hopping strengths. This is a simple consequence of the Wannier function being an odd function of the coordinate normal to the nodal plane, as well as having a wider extension along that direction. This is also implied by the familiar bandstructures in a one-dimensional system where their lowest band has a minimum at $k = 0$ while the first excited band has a minimum at the edge of the Brillouin zone.

Because of the strong anisotropy of the excited band tunneling strengths, the structure of the ideal gas Fermi surface is quite unlike that in the lowest band. In the lowest band, the Fermi surface is roughly spherical for low filling fractions, but on the excited bands Fermi surfaces are more sheet-like since atoms first fill the states along the directions perpendicular to the direction of large tunneling strength. The Hamiltonian we derived is very rich and the possible phases that can occur in different parameter regimes are numerous. We now proceed to discuss a few applications. First, we discuss anti-ferromagnetic phases with repulsive interactions and then we proceed to discuss the paired phases with attractive interactions.

### III. Repulsive Interactions

The order parameter for an antiferromagnetic state with an ordering vector $\mathbf{Q}$ is defined as $A_{\alpha,\mathbf{Q},\sigma} = V^{-1} \sum_{\mathbf{k}} (\psi_{\alpha,\mathbf{k}+\mathbf{Q},\sigma}^\dagger \psi_{\alpha,\mathbf{k},\sigma})$, where $V$ is the dimensionless volume, i.e., the total number of sites in the system. In principle, two types of antiferromagnetic state are conceivable in the repulsive case: either one with checkerboard symmetry, so that $\mathbf{Q} = (\pi, \pi, \pi)$ in Cartesian coordinates, or a striped phase where symmetry is broken,
Q = (π, 0, 0). However, as we shall see, the striped phase is found to be energetically unfavorable. Following Ref. [23], the interaction part of the Hamiltonian is written in a mean-field approximation as

\[ H'_1 = \sum_{\alpha k} U_{1,\alpha} n_{\alpha 0} \left( \psi^{\dagger}_{\alpha,\mathbf{k}} \psi_{\alpha,\mathbf{k}} + \psi^{\dagger}_{\alpha,\mathbf{k} + \mathbf{Q}_1} \psi_{\alpha,\mathbf{k} + \mathbf{Q}_1} \right) + U_{1,\alpha} n_{\alpha 1} \left( \psi^{\dagger}_{\alpha,\mathbf{k}} \psi_{\alpha,\mathbf{k}} + \psi^{\dagger}_{\alpha,\mathbf{k} + \mathbf{Q}_1} \psi_{\alpha,\mathbf{k} + \mathbf{Q}_1} \right) + U_{1,\alpha} A_{0,\mathbf{Q}_1} \left( \psi^{\dagger}_{\alpha,\mathbf{k} + \mathbf{Q}_1} \psi_{\alpha,\mathbf{k}} + \text{h.c.} \right) + U_{1,\alpha} A_{0,\mathbf{Q}_1} \left( \psi^{\dagger}_{\alpha,\mathbf{k}} \psi_{\alpha,\mathbf{k}} + \text{h.c.} \right) - V \sum_{\alpha} U_{1,\alpha} (n_{\alpha 0} n_{\alpha 1} + A_{0,\mathbf{Q}_1} A_{\mathbf{Q}_1}), \] (3)

where the primed sum extends only over the reduced Brillouin zone (RBZ), defined such that the points \{\bm{k}, \bm{k} + \mathbf{Q} | \mathbf{k} \in \text{RBZ}\} make up the first Brillouin zone. The quantities \( n_{\alpha 0} \) and \( n_{\alpha 1} \) are the densities of the components occupying the respective orbitals. A Bogoliubov transformation diagonalizes the Hamiltonian, whereafter the free energy \( \Omega(A_{0,\mathbf{Q}_1}, A_{x,\mathbf{Q}_1}, A_{y,\mathbf{Q}_1}, A_{z,\mathbf{Q}_1}) = -k_B T \log[\text{Tr} \exp[-\beta (H_{\text{ideal}} + H'_1)]] \) can be computed. Here, \( \beta = 1/(k_B T) \), and \( T \) is the temperature. For definiteness, we assume that both components experience the same lattice potential and that the lattice potential has the same depth in all directions. Parameters are calculated for \(^{40}\text{K}\) atoms in a lattice of depth \( V_0 = 8 E_R \), where \( E_R \) is the recoil energy of the atoms when they absorb a photon (of wavelength 826 nm). In that case, we obtain \( J_0 = 0.012E_R \), \( J_{1,\alpha} = -0.15E_R \), and \( J_{1,3} = 0.0028E_R \) if \( \alpha \neq \beta \), which demonstrates our earlier qualitative arguments about the magnitude of the tunneling terms. For \( a = 174 \) Bohr radii, \( U_0 = 0.30E_R \) [24]. We assume that using a magnetic field \( a \) can be tuned to arbitrary positive at negative values [1].

As \( a \) is increased, the system undergoes a first-order transition from the normal state, with \( A_{0,\mathbf{Q}_1} = 0 \) for all \( \alpha \), to a checkerboard state where \( A_{0,\mathbf{Q}_1} \neq 0 \) and \( A_{x,\mathbf{Q}_1} = A_{y,\mathbf{Q}_1} = A_{z,\mathbf{Q}_1} \). The order parameter \( A_{x,\mathbf{Q}_1} \) is plotted in Fig. 1. The magnitude of \( A_{0,\mathbf{Q}_1} \) displays a similar behavior. The chemical potentials are in the calculation fixed to \( \mu_1 = 6J_{0,1} \) and \( \mu_1 = \Delta_{x,\text{BG}} + 2(J_{xy} + J_{xz}) \), respectively: this is in the noninteracting limit close to the value for half-filling. The phase diagram is found to be very insensitive to the exact values of the chemical potentials; in the antiferromagnetic state, the densities are locked to the values \( n_1 = 0.5 \) and \( n_1 = 1.5 \), respectively, so that for the majority component, the mean occupation of the 0 orbital is unity and the combined occupation of the \( x, y, \) and \( z \) orbitals is 0.5. If the fermions are confined in a magnetic trap, the state of the system is to a good approximation given by a local-density approximation where the local chemical potential is given by the sum of the chemical potential and the negative of the trapping potential. The fact that the state of the system is insensitive to the chemical potential then means that without much fine-tuning, the antiferromagnetic state can be made to occupy a large area in the trap, with corrections only toward the edges where the density drops to zero.

A fully antiferromagnetic state, where the occupations of neighboring states in each spin state alternates between 0 and 1, has an order parameter of magnitude exactly equal to 0.5. It is seen in Fig. 1 that the system in the checkerboard state is always close to this limit because of the strong repulsive interactions. The absence of a stripped phase in these calculations is not conclusive proof that such a state is always thermodynamically unfavorable. On the contrary, it is conceivable that stripped phases could show up, e.g., in anisotropic lattices or in lower dimensions. For the parameter ranges that we investigated here, the checkerboard state always has the lower free energy.

**IV. ATTRACTIVE INTERACTIONS**

In order to study BCS-type paired states with attractive interactions (i.e., negative \( a \)), we introduce auxiliary (pairing) fields \( \Delta_0 = U_0 \langle \psi_{0,i,1} \psi_{0,i,1} \rangle \) and \( \Delta_\alpha = U_{1,\alpha} \langle \psi_{0,i,1} \psi_{0,i,1} \rangle \) which we use to decouple the interaction terms in the usual way. In this way we find the interaction term of the mean-field Hamiltonian

\[ H_1'' = \sum_i \Delta_0 \psi^{\dagger}_{0,i,1} \psi_{0,i,1} + \Delta_0 \psi_{0,i,1} \psi_{0,i,1} - |\Delta_0|^2/U_0 \]

\[ + \sum_{\alpha,i} \Delta_\alpha \psi^{\dagger}_{0,i,1} \psi_{0,i,1} + \Delta_\alpha \psi_{0,i,1} \psi_{0,i,1} - |\Delta_\alpha|^2/U_{1,\alpha} \]

The Hamiltonian is then diagonalized with a canonical transformation and the grand potential computed and minimized in order to find the state that is physically realized.
all pairing fields are equal, i.e., $\Delta_x = 0$, and the minority component chemical potential which corresponds to half-filling for the ideal system at $T = 0$. The $x$-axis shows the filling fraction of the ideal gas of majority atoms at $T = 0$. Shading: symmetric state = light, on-axis state = gray, normal state = dark.

In Fig. 2 we show an example phase diagram when the minority component chemical potential is fixed to the value corresponding to half-filling for an ideal Fermi gas at $T = 0$ and the majority component chemical potential and temperature are varied. The lattice parameters were chosen the same as before. For the assumed symmetric lattice we can identify three different phases: the normal state where all pairing fields vanish, the on-axis state where only one $\Delta_x \neq 0$, and the symmetric state where all pairing fields are equal, i.e., $\Delta_x = \Delta_y = \Delta_z$. The last one of these states dominates at low temperatures and for lower majority component filling factors. The on-axis state can be favorable at low temperatures and somewhat higher filling factors, while the normal state is favorable elsewhere. It should be noted, that whether or not the on-axis state appears depends also on the coupling strength. If the coupling is increased, the symmetric state with equal pairing fields occurs on a larger part of the phase diagram.

From our computations (not shown in the figures) we observe the presence of a critical coupling strength before pairing can take place. The reason for the critical coupling strength has to do with a different structure of the Fermi surfaces of the majority and minority atoms. For identical atoms at the lowest band the Fermi surfaces can be perfectly matched for zero polarization, but this is no longer true when one of the components occupies states on the excited $p$-bands. In this case sufficiently strong coupling is required to counteract the effect of the mismatched Fermi surfaces. Just above the critical coupling strength the on-axis state has a slightly lower energy than the symmetric state while for stronger couplings the latter state is favored.

V. CONCLUSIONS

 Optical lattice experiments usually include a parabolic trapping potential. When one starts to increase the number of majority atoms while keeping the number of minority atoms fixed, the higher bands will not be occupied straight away. At first, the cloud of majority atoms spreads out in the harmonic trap and their filling factor in the optical lattice remains less than one. However, roughly at distances larger than $R$ the energy $m\omega_T^2 R^2/2$ due to the trapping potential with frequency $\omega_T$ becomes larger than the bandgap. When this happens, it is favorable for the atoms to start filling the excited band(s) in the center of the trap. This implies that in a trapping environment the phases discussed in this paper can occur in the center of the atomic cloud and that this center will be surrounded by a cloud of majority atoms occupying the lowest band. The presence of the pairing gaps and anti-ferromagnetic ordering would be observable, for example, through noise-correlation experiments \cite{25, 26, 27}. In the noise correlation experiments the structure of the correlation peaks will depend on the symmetry of initial Wannier functions of the atoms prior to free expansion and can therefore be used to distinguish various phases. Pairing gaps could also be observed through radio-frequency spectroscopy \cite{28, 29, 30}.

In this article we derived a theory for the two-component polarized fermions in an optical lattice when also the lowest excited $p$-bands are occupied. Based on this theory we studied anti-ferromagnetic phases as well as mean-field BCS-type theory with several possible order parameters. We outlined the expected phase boundaries for anti-ferromagnetic phases, whose properties need to be studied in greater detail in the future. In the attractive case we assumed BCS order parameters which do not break translational symmetry, thus postponing the investigation of states which do break the translational symmetry in a lattice \cite{7, 31}. Interesting physics is also expected when the minority component starts to populate the excited bands. In this case one can expect competition between inter-band and intra-band effects.

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