Cyclic Lattice Feshbach Resonances

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In this Letter we illustrate the possible cyclic fermion pairing states across Feshbach resonances in optical lattices. In cyclic fermion pairing, the pairing amplitude exhibits an oscillatory behavior as the detuning varies. We estimate the quasi-particle gaps in different regimes of the resonances.

Feshbach resonances in optical lattices were recently investigated in experiments[1, 2], after the earlier observation of Feshbach resonances in traps[3-6]. The fascinating phenomenon of lattice Feshbach resonances (LFRs) has attracted a lot of attention; both many-body physics and few-body aspects across LFRs have been studied[7, 8, 9, 10, 11]. Across LFRs fermionic atoms were observed to form shallow molecules, and superfluids should be present in optical lattices when tunneling is permitted[2]. However, superfluids in LFRs can exhibit distinct properties. For instance, repulsive interactions between molecules[12], which have usually been overlooked in standard theoretical studies of superfluids near Feshbach resonances in traps, play a significant role in LFRs; the superfluid long-range-order can be substantially renormalized by these interactions[13].

In this Letter, we study the pairing between fermions near LFRs, taking into account repulsive interactions between bosonic molecules in the closed channel. We show that in the limit of large repulsive interactions between molecules, or small molecule band width, LFRs should exhibit a cyclic behavior as the detuning varies. Namely, the fermion quasi-particle energy gaps and critical temperatures of superfluids across LFRs exhibit an oscillatory behavior; the gap reaches maxima in a hard-core boson limit.

Consider the following Fermi-Bose lattice model:

\[
H = H_f + H_b + H_{bf};
\]

\[
H_f = \sum_{<kl>, \eta, \eta', \sigma} t_{f, \eta \eta'} (f_{k \eta \sigma}^\dagger f_{l \eta' \sigma} + h.c.) + \sum_{k, \eta, \sigma} (\epsilon_\eta - \mu) f_{k \eta \sigma}^\dagger f_{k \eta \sigma}
\]

\[
H_b = -t_b \sum_{<kl>} (b_{k \eta}^\dagger b_{l \eta} + h.c.) + \sum_k (2v - 2\mu) b_{k \eta}^\dagger b_{k \eta} + U_b \sum_k \hat{n}_{b \eta} (\hat{n}_{b \eta} - 1);
\]

\[
H_{bf} = -\gamma_0 \sum_{k, \eta, \eta'} g_{\eta \eta'} (b_{k \eta}^\dagger f_{k \eta \eta'} f_{k \eta' \dagger} + h.c.)
\]

Here \(k, \eta\) and \(\sigma\) label lattice sites, on-site orbitals and spins; \(\eta = 1, 2, ..., M\), \(\sigma = \uparrow, \downarrow\). \(f_{k \eta \sigma}\) (\(f_{k \eta \eta'}\)) is the creation (annihilation) operator of a molecule (fermion) at site \(k\), with on-site orbital energy \(\epsilon_\eta\) and spin \(\sigma\). \(b_{k \eta}^\dagger (b_{k \eta})\) is the creation (annihilation) operator of a molecule (fermion) at site \(k\) (For simplicity, We assume there is only one bosonic orbital degree of freedom at each site). The boson number operator is \(\hat{n}_{b \eta} = b_{k \eta}^\dagger b_{k \eta}\). \(t_{f, \eta \eta'}\) and \(t_b\) are hopping integrals of fermions and bosons respectively and hopping occurs over neighboring sites labeled as < \(kl\) >. The single particle tunneling of bosons in optical lattices is assumed to be small, so that \(t_b\) is much less than \(U_b\), the on-site repulsive interaction between bosonic molecules; \(t_f\) is much larger than the energy difference between two orbitals. \(H_b\) is the Hamiltonian previously introduced for atoms in optical lattices[14]; it has been used to study Mott insulator-superfluid phase transitions which were recently observed in optical lattices[15].

Finally in narrow resonances, or in the large-N limit treated before[13], the matrix \(g_{\eta \eta'}\) is proportional to \(\delta_{\eta \eta'}\). However, in other limits the \(g\)-matrix generally has off-diagonal terms[10]. Here we assume \(g_{\eta \eta'}\) to be an arbitrary symmetric matrix so that the spatial wavefunction of pairs is symmetric and spin wavefunction antisymmetric.

The self-consistent chemical potential is determined by the following formula,

\[
N = 2N_b (2\mu - 2v; t_b, U_b; \lambda_b (\gamma_0, t_f, \mu)) + N_f (\mu; t_f; \lambda_f (\gamma_0, t_b, U_b))
\]

where \(N\), \(N_b\) and \(N_f\) are, respectively, the total number of fermions, the number of molecules or bound states of atoms and the number of atoms per lattice site. \(\lambda_f (b)\) is the effective interaction constant between fermionic atoms(molecules) mediated by molecules (fermions). We are interested in the limit where the coupling strength \(\gamma_0\) is small compared with \(U_b\) so that in the calculation of \(N_b (N_f)\) we can neglect the \(\lambda_b (\lambda_f)\)-dependence.

When \(t_b\) is much smaller than \(U_b\), molecules can be considered to be in a Mott insulating ground state to the zeroth order in \(\gamma_0 10\). Therefore \(N_b\) is a step-like function of the detuning \(v\). In the limit of zero \(t_b\), \(N_b\) is equal to an integer \(n\) whenever \(2\mu - 2v - U_b - I < 1/2\); \(N_b\) has two degenerate solutions when \(2\mu - 2v - U_b = I + 1/2\) and the value of \(N_b\) jumps from \(I\) to \(I + 1\) at that particular detuning signifying a discontinuous transition between two plateaus in the \(N_b\) versus \(v\) curve.
transition from the geral structure of the step-like function, except that the\[ X \in (a) \] is when the band and the bottom of the lowest molecule Mott band is the atomic band. The distance from the bottom of the atomic bands and empty lobes for unfilled Mott bands; the partially shaded lobes stand for completely filled molecular Mott bands. The distance from the bottom of the atomic band and the bottom of the lowest molecule Mott band is the detuning \(|v|\).

A finite but small value of \(t_b\) won’t change the general structure of the step-like function, except that the transition from the \(I\)th plateau to the \((I+1)\)th plateau becomes smooth. Generally, we have

\[
N_b(2\mu - 2v; t_b, U_b) = Int\left(\frac{2\mu - 2v - Int(2\mu - v/U_b)U_b}{2zt_b} + 1\right),
\]

\[F(X) = \begin{cases} 1, & 1 \leq X < \frac{\mu - v}{zt_b}; \\ f(X), & 0 \leq X \leq 1; \\ 0, & -\frac{U_b}{zt_b} \leq X \leq 0. \end{cases}\]  

Here \(IntY = I\) if \(-1/2 \leq Y - I < 1/2\); \(X\) is the distance (in energy space as shown in Fig.1) from the chemical potential to the bottom of the nearest Mott band measured in the unit of \(2zt_b\) (where \(z\) is the coordination number). The filling factor \(f(X)\) is a continuous function of \(X\) varying from 0 at \(X = 0\) to one at \(X = 1\). Its detailed form depends on the band structure, which is not specified here.

Taking into account this general property of \(N_b\), one easily finds that the solution to Eq. (2) is also a step-like function of \(v\) (see Fig. 2). Whenever the detuning is such that \(-\frac{U_b}{zt_b} < X \leq 0\) or \(1 \leq X < \frac{\mu - v}{zt_b}\), varying the detuning \(v\) does not change \(N_b\) or \(N_f\) and therefore the chemical potential for fermions must be a constant. This leads to plateaus in the self-consistent chemical potential. The first plateau represents the limit of extremely weakly interacting superfluids, i.e. the detuning is positive and much larger than the fermion energy of atoms. The chemical potential in this limit barely depends on the detuning \(v\) or coupling constant \(\gamma\); its value is approximately equal to the Fermi energy of a noninteracting Fermi gas, i.e. \(\mu_1 \approx \epsilon_F\); \(\epsilon_F\) is the Fermi energy of a gas with \(N\) atoms per site. The value of the chemical
potential on the $i$th plateau is given as

$$
\mu_i = \mu_{i-1}^{3/2} - (i-1) (\epsilon_F^{0})^{3/2}, i \leq i_{\text{max}}
$$

where $\epsilon_F^{0}$ is the Fermi energy of an atomic gas with two atoms per lattice site. The number of plateaus in the chemical potential $i_{\text{max}}$ is determined by the density of atoms; for $N/2 = n + \epsilon$ (a is an integer and $0 < \epsilon < 1$), the value of $i_{\text{max}}$ and the number of valleys in Fig.2(b) are $n + 1$.

The transition between two plateaus takes place when the self-consistent chemical potential is located inside a Mott band; i.e. when $X$ is between zero and one. The width of the transition region when the detuning varies is proportional to the band width $2zt_b$. The distance between two consecutive transition regions is $v_{i+1} = U_k; v_i$ is the detuning at the $i$th transition region when $X(v_i) = 1/2$.

The trial wavefunction for the fermion sector is

$$
|\text{g.s.}> = \prod_{\mathbf{q}} \left[ u(\mathbf{q}) + v_{\eta \xi}(\mathbf{q}) f_{\eta \xi}(\mathbf{q}) f_{\eta \xi}^{\dagger}(-\mathbf{q}) \right]|0>.
$$

$q$ is the crystal quasi-momentum and $u^2 + \sum_{\eta \xi} v_{\eta \xi}^2 = 1$.

The solutions when chemical potentials are located on a plateau are distinctly different from the solutions when the chemical potentials are in a smooth transition region (Fig.2(a)). We will discuss these two limits separately. When $X$ (defined in Eq.(3)) is either larger than unity or smaller than zero, the chemical potential falls on a plateau. Unoccupied molecule states, with which fermions in extended states have resonances, are well above the self-consistent chemical potential. The difference between the energy of the lowest molecule state and the chemical potential depends on the detuning $\nu$ or $X$. The energy difference $2\delta_1(X)zt_b(>0)$ is equal to $2Xzt_b$ if $0 > X > -U_b/4zt_b$ and equal to $U_b - 2Xzt_b$ if $1 < X < U_b/4zt_b$; typically it is a fraction of $U_b$. When $\delta_2(X) > 1$, one obtains the effective on-site attractive interaction between atoms mediated by molecules

$$
V_{\eta \xi, \eta' \xi'} = -\lambda_f g_{\eta \xi} g_{\eta' \xi'}, \lambda_f = \frac{\gamma_0^2}{2 \delta_1(X)zt_b}.
$$

Minimization of the free energy $< \mathcal{H} > - \mu N$ leads to the following equations for $(u, v_{\eta \xi})(V$ is the volume):

$$
\begin{align*}
2uv_{\eta \xi} \xi'_{\eta'}(\mathbf{q}) &= \Delta(\delta_{\eta \xi} u^2 - \delta_{\eta' \xi'} v_{\eta' \xi'} v_{\eta \xi}); \\
\Delta &= \frac{\lambda_f}{V} \sum_{\mathbf{q},\eta, \xi} g_{\eta \xi} v_{\eta \xi}(\mathbf{q}) u(\mathbf{q}).
\end{align*}
$$

Here $\xi_{\eta' \eta}(\mathbf{q}) = \epsilon_{\eta' \eta}(\mathbf{q}) - \mu$, $\epsilon_{\eta' \eta}$ is the kinetic energy tensor. The lattice constant has been set to unity.

Solutions to this equation depend on the details of $g_{\eta \xi}$ and the dispersion $\xi_{\eta' \eta}(\mathbf{q})$. In the limit when the different bands are degenerate, i.e. $\xi_{\eta' \eta}(\mathbf{q}) = \delta_{\eta' \eta} \xi(\mathbf{q})$, one obtains $v_{\eta \xi} = g_{\eta \xi} v_u$; $(u, v)$ are the usual BCS solutions,

$$
\frac{2uv}{u^2 - v^2} = \frac{\Delta}{\xi(\mathbf{q})}; \\
\frac{V}{\lambda_f} = \sum_{\mathbf{q}} \frac{1}{2E(\mathbf{q})} - \sum_{\mathbf{q}} \frac{1}{2\epsilon(\mathbf{q})}.
$$

Here $E(\mathbf{q}) = \sqrt{\xi^2(\mathbf{q})} + |\Delta|^2$ is the quasi-particle energy; $\sum_{\eta' \eta} g_{\eta' \eta}^2 = 1$. The energy gap $\Delta \sim t_f \exp(-2/\lambda_f)$ is exponentially small. $\lambda_f$ is a dimensionless interaction constant estimated to be $C \frac{\gamma_0^2 N_b^{1/3}}{\sigma}$; we have assumed the atomic density of states at the chemical potential is $CN_b^{1/3}/tf$. $C$ is a quantity of order unity which depends on the details of the band structure.

When $0 \leq X \leq 1$, the chemical potential is between two plateaus and varies continuously as a function of $X$ within this window. In the mean field approximation one obtains the following modified self-consistent equation, $\Delta = \gamma_0 < b >, -\delta_2(X)2zt_b + \lambda < b > = \gamma_0^2 \sum_{\mathbf{q}} \left( 1/2E(\mathbf{q}) - 1/2\epsilon(\mathbf{q}) \right); \lambda(U_b)$ is an interaction constant appearing in an effective theory and is of order of $U_b$.

When the chemical potential $\lambda(U_b)N_b$ becomes comparable to the Fermi energy of a Fermi gas with the corresponding density (which scales as $N_b^{2/3}zt_b$), the mean field approach fails; this sets the limit on the number of atoms per lattice site, which has to be much less than $(zt_b/U_b)^3$. The window where mean field theory is applicable thus shrinks to zero as $zt_b/U_b$ approaches zero.

To get an estimate of $b >$ in the large-$U_b$ limit, it is useful to map the model to an XXZ model. Since the completely filled Mott bands are irrelevant to the discussions of superfluids, we only need to take into account the partially filled band. When $t_b$ is much less than $U_b$, the molecules can be treated as hard-core bosons at energy scales much lower than $U_b$. For hard-core bosons, the on-site Hilbert space is one boson and no bosons. The average number of bosons at each lattice site varies from zero to one depending on the position of chemical potentials.

This suggests an effective pseudo spin $S = 1/2$ subspace (on-site): $|\sigma_k^z\rangle = -1 \equiv b_k^{\dagger} |\text{vac} > b_k$, $|\sigma_k^z = 1 \equiv |\text{vac} > b_k$. $|\text{vac} > b_k$ is the vacuum of bosons. Furthermore, in this truncated space one can easily verify that three Pauli matrices can be represented as $\sigma_k^z = 1 \equiv 2b_k^{\dagger} b_k, \sigma_k^x \equiv b_k^{\dagger} \rightarrow b_k$ and $\sigma^- \equiv b_k^{\dagger}; \sigma_\pm = (\sigma^x \pm i\sigma_y)/2\sqrt{2}.$

A state with $\sigma_k^z = 1$ corresponds to a vacuum of molecules, and $\sigma_k^z = -1$ a Mott state with one molecule.
per lattice site. On the other hand, in translationally invariant states where $\sigma_k$ has a finite expectation value in the $XY$ plane, the condensation amplitude of molecules is nonzero; i.e.

$$\langle b_k \rangle = \langle \sigma_k^- \rangle . \quad (9)$$

So any state with all $\langle \sigma_k \rangle$ pointing along a specified direction that differs from the $z$-axis breaks the in-plane ($XY$ type) rotational symmetry of the pseudo spin and corresponds to a superfluid. The effective Hamiltonian for molecules can then be written as

$$H_{\text{eff}} = -\frac{t_b}{2} \sum_{\langle kl \rangle} \sigma_k^x \sigma_l^x + \sigma_k^y \sigma_l^y + \hbar \gamma \sum_k \sigma_k^z. \quad (10)$$

Here $\hbar \gamma = (X - 1/2)2zt_b$. The Hamiltonian is invariant under a rotation around the $z$-axis or has an XY symmetry which corresponds to the usual $U(1)$ symmetry of a boson field.

One easily finds the ground state of the above Hamiltonian using a semiclassical approximation \[18\] and gains insight into superfluids in the large-$U_b$ limit. In the semiclassical approximation, one assumes that the orientation of a pseudo spin is specified by a polar angle $\Theta$ and an azimuthal angle $\Phi$ as: $\langle \sigma^x \rangle = \sin \Theta \cos \Phi$, $\langle \sigma^y \rangle = \sin \Theta \sin \Phi$ and $\langle \sigma^z \rangle = \cos \Theta$.

Minimizing the mean field energy with respect to $\Theta$ leads to the following solution for $\Theta$. $\Theta$ remains at 0 as $X$ becomes negative, corresponding to an empty Mott band. As $X$ becomes larger than 1, $\Theta$ is equal to $\pi$ representing a Mott state with one molecule per site. For $1 > X > 0$, one obtains $\cos \Theta = 1 - 2X$, or $\sin \Theta = 2\sqrt{X(1-X)}$; note that in this limit all solutions with a given $\Theta$ but arbitrary $\Phi$ are degenerate and break the usual $U(1)$ symmetry of a superfluid. Following Eq.(9) and Eq.(10), one arrives at $\Delta = \gamma_0 \sin \Theta \exp(-i\Phi)$, or in terms of $X$

$$\Delta = \gamma_0 2\sqrt{X(1-X)} \exp(-i\Phi). \quad (11)$$

At $X = 1/2$ or half filling, $\sin \Theta = 1$ and the modulus of the expectation value $\langle b \rangle$ (proportional to $\sin \Theta$) reaches its maximum. This leads to the maximal value of the BCS gap, $|\Delta| = \gamma_0$.

The calculation of $T_c$ in the large $U_b$ limit is tricky because of large quantum fluctuations present when the chemical potential falls in the middle of a Mott band. Here we estimate $T_c$ again in two limits: a) when the chemical potential falls on a plateau corresponding to various valleys in Fig.\[2\](b); b) when the chemical potential is between two plateaus. In case a), fermions are weakly interacting and we expect the BCS theory to be valid. $T_c$ scales as $\Delta$, the solution to Eq.(8) and is exponentially small when $\gamma_0$ is much smaller compared to $U_b$. In case b), $T_c$ should be approximately the BEC transition temperature of molecules in a partially filled Mott band, which is proportional to $e^{2/3}\gamma t_f$ ($\epsilon(<1)$ is the filling fraction.). This temperature differs from the quasi-particle gap calculated in Eq.\[11\] and is also independent of the coupling constant $\gamma_0$. It reaches a maximal value when $X = 1/2$ because of the particle-hole symmetry. Therefore, we expect an oscillatory behavior in the critical temperature as well. At a temperature lower than the BEC temperature but higher than the exponentially small BCS transition temperature when the chemical potential is between two Mott bands, the ground state is expected to alternate between a fermionic superfluid and a normal fluid as the detuning is varied. This might be observed in future experiments on LFRs. I would like to thank T. Leggett, K. Madison and G. Warner for discussions. This work is supported by a grant from UBC, a Discovery grant from NSERC, Canada and by the A. P. Sloan foundation.

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\[14\] D. Jaksch et al., Phys. Rev. Lett. \textbf{81}, 3108 (1998) and references therein.
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\[16\] Strictly speaking, molecular Mott states are not well-defined in the presence of resonances between fermion atoms and bosonic molecules. See more discussions in Ref.\[2\] \[18\]. However, in the current situation, we find the induced condensation fraction in a molecular Mott state is of order of $(\gamma_0/U_b) \exp(-2/\lambda f)$ and for practical reasons we neglect such a contribution in our calculations because $U_b$ is assumed to be much larger than $\gamma_0$.

\[17\] In this limit, the interactions between atoms mediated by molecules are negligible so that at a given chemical potential, we can neglect the $v$-dependence in the calculation of $N_f$.

\[18\] Similar calculations can be found in F. Zhou et al., Phys. Rev. B \textbf{70}, 184434 (2004).