Pairing with Unconventional Symmetry around BCS-BEC Crossover: Fermionic Atoms in 2D Optical Lattices to Correlated Electron Systems

Dušan Volčko and Khandker F. Quader

Department of Physics, Kent State University, Kent, OH 44242

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We study superfluid properties of fermions on a 2D lattice using a finite-range pairing interaction derivable from an extended Hubbard model. We obtain signatures of unconventional pair-symmetry states, $d_{x^2-y^2}$ and extended-s ($s^*$), in the BCS-BEC crossover region. The fermion momentum distribution function, $v_F^2$, the ratio of the Bogoliubov coefficients, $v_k/u_k$, and the Fourier transform of $v_F^2$ are among the properties that are strikingly different for $d$- and $s^*$ symmetries in the crossover region. Fermionic atoms in 2D optical lattices may provide a way to observe these signatures. We discuss possible experimental ramifications of our results.

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Attainment of boson and fermion condensates [1] of ultracold neutral atoms has presented an unprecedented opportunity to study properties of quantum many-particle systems. Fermionic atoms in optical lattices [2, 3] constitute yet another intriguing set of systems. While these are by themselves interesting to study, they may also provide a way to gain useful insight into properties of correlated electrons in solids. Jaksch et al [4] suggested that atoms in optical lattices, confined to the lowest Bloch band, can be represented by the Hubbard model with hopping kinetic energy $t$ between neighboring sites, and on-site interaction $U$. Hubbard model calculations [5, 6, 7] predict that attractive-U Hubbard model give rise to s-wave superconductivity, while the repulsive-U model results in an antiferromagnetic or a d-wave superconducting phase depending on filling (number of fermions per lattice site). Owing to the continuous tunability of model parameters such as, density, hopping or interactions, optical lattices can serve as testing grounds for such models. This has led, for example, to the suggestion [5] that the underlying physics of the high $T_c$ superconductors may be understood by studying these systems. Recent work [2, 3, 10] have pointed out possible role of additional Bloch bands and multi-band couplings in optical lattices. In solids this would correspond to having multiple orbitals and near-neighbor interactions. Duan [9] has shown that on different sides of a broad Feshbach resonance, the effective Hamiltonian can be reduced to a t-J model, familiar in correlated electron systems, wherein it has been suggested [7] that t-J model can give rise to d-wave pairing.

Fermionic atoms subjected to positive and negative detuning using Feshbach resonance technique provide realizations of BEC-BCS crossover behavior. It has been recently suggested [11] that it should also be possible to study superfluid properties of fermions in optical lattices around BEC-BCS crossover regime. Starting with the seminal work of Eagles [12] and Leggett [13], the BEC-BCS crossover problem received considerable theoretical attention [5, 14, 15, 16, 17, 18, 19] due to the possibility that high $T_c$ superconductors, possessing short coherence lengths, could fall in the BEC-BCS crossover region. Several authors employed continuum models [5, 14, 15, 16, 19], focussing mostly on conventional s-wave pair symmetry. Lattice models with on-site or nearest-neighbor attractions have also been considered [5, 14, 17, 18, 19]. More recent theory work [20] are in the context of cold fermions.

Motivated by these issues, in this paper, we study superfluid properties of fermions in a 2D square lattice in the BEC-BCS crossover regime using a finite-range pairing interaction, obtainable from a multi-band extended Hubbard model. As representative cases of unconventional pair symmetry, we consider two even-parity representations of the cubic group, namely the $\ell = 2$ $d_{x^2-y^2}$-wave, and the $\ell = 0$ extended s-wave ($s^*$). There has been work [18, 19, 21] employing similar pairing interaction; however these have focussed on different systems and issues. We present several new results, including specific signatures of superfluid states with unconventional pairing gap symmetry as one goes between the BEC and BCS regimes. This could provide a way to distinguish between different gap symmetry states in systems that allow for tuning into the BEC-BCS crossover regime, such as fermionic atoms in 2D optical lattices, and possibly high $T_c$ cuprates. One of our key results is the remarkable behavior of the fermion distribution function, $v_F^2$, (related to momentum distribution, $u_k$): For the d-wave gap function, $v_F^2$ changes abruptly from having a peak at the Brillouin zone (BZ) center $(0,0)$ to a vanishing central peak accompanied by a redistribution of the weight around other parts of the BZ $((0, \pm \pi), (\pm \pi, 0))$ as the system crosses from the weak-coupling BCS to the strong-coupling BEC regime. By contrast, $v_F^2$ changes smoothly in the $s^*$-wave case. Similar signatures are also found in the ratio of Bogoliubov coefficients $v_k/u_k$, related to the phase of the superfluid wavefunction. The Fourier transform of $v_F^2$ in real space exhibits a “checkerboard” type pattern that could have consequences for experiments.

The extended Hubbard model for two equal species of fermions with $\ell = 0$, $\pm 2$ and $s^*$, $d_{x^2-y^2}$ pairing is given by

$$H = -t \sum_{\langle \mathbf{r}, \mathbf{r} \prime \rangle} \sum_{\sigma} c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r} \prime, \sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}, \uparrow} n_{\mathbf{r}, \downarrow} - \mu \sum_{\mathbf{r}, \sigma} n_{\mathbf{r}, \sigma},$$

where $c_{\mathbf{r}, \sigma}$ is the fermion field operator at site $\mathbf{r}$ and spin $\sigma$, $n_{\mathbf{r}, \sigma} = c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}, \sigma}$ is the fermion occupation number, $\mu$ is the chemical potential, $t$ is the hopping integral, and $U$ is the on-site interaction. The terms $U n_{\mathbf{r}, \uparrow} n_{\mathbf{r}, \downarrow}$ represent on-site repulsions.

The ground state of the model is given by the Bogoliubov dispersion relation

$$\omega_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + v_F^2} = \sqrt{\epsilon_{\mathbf{k}}^2 + \left(\frac{\hbar^2}{2m^*}\right) k^2 v_F^2},$$

where $\epsilon_{\mathbf{k}}$ is the momentum $k$ is the momentum of the Bloch state, $\hbar$ is the reduced Planck constant, and $m^*$ is the effective mass.

The Bogoliubov coefficients $v_k$ are related to the momentum distribution function $u_k$ by

$$u_k = \frac{1}{\sqrt{2 \pi}} \frac{1}{v_k},$$

With the Bogoliubov coefficients, the Fourier transform of the superfluid wavefunction can be written as

$$\psi_{\mathbf{k}} = \sum_{\mathbf{k}'} v_{\mathbf{k}-\mathbf{k}'} \psi_{\mathbf{k}'}.$$

For $d_{x^2-y^2}$ pairing, the wavefunction has a $d$-wave pattern, while for $s^*$ pairing, it has a $s^*$-wave pattern.

The extension of this model to include additional bands and multi-band couplings is straightforward and allows for a rich variety of quantum many-body phenomena. This model is particularly relevant to the study of cold fermions in optical lattices, where it can provide insights into the superfluid properties of these systems. The possibility of realizing unconventional superfluid states, such as those associated with $d_{x^2-y^2}$ and $s^*$ wave symmetries, opens up new avenues for experimental exploration and theoretical understanding.

We conclude by emphasizing the potential of this model as a platform for the study of unconventional superfluid states in cold fermionic systems. The ability to tune the model parameters, such as the hopping integral and on-site interactions, offers a unique opportunity to explore the full range of quantum many-body phenomena in these systems. The results presented here highlight the rich physics that can be uncovered by studying these models, and we look forward to future experimental and theoretical advances in this exciting field.
population system on a 2D square lattice is given by:

\[ H = \sum_{<ij>,\sigma} (-tc_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\sigma} n_{i\bar{\sigma}} - V \sum_{<ij>,\sigma\sigma'} n_{i\sigma} n_{j\sigma'} - \mu_o \sum_i n_i, \tag{1} \]

where \( t \) is the kinetic energy hopping, \( \mu_o \) the unrenormalized chemical potential, \( U \) the on-site repulsion and \( V \) the nearest-neighbor attraction. In the case of cold fermions on a lattice, \( V \) would be related to inter-band coupling. \( \sigma \) is the “pseudo-spin” index, that could refer to equally populated hyperfine states in the case of optical lattices. At the mean-field level, the Hartree self-energy terms renormalize \( \mu_o \) such that \( \mu = \mu_o + \mu_U(f) + \mu_V(f) \) where \( \mu_U(f) \) and \( \mu_V(f) \) are filling-dependent corrections to \( \mu \).

We work with the renormalized \( \mu \) so as to properly deal with weak and strong couplings, and take \( \mu_{j,f}(f) = J_f f \), where \( J_f = U, -V \). The filling \( f = N/2M \), with \( N \) the number of particles, \( M \) the number of lattice sites, and the pseudo-spin degeneracy factor 2. On Fourier transforming and retaining interactions between particles with equal and opposite momentum, as in BCS theory, the reduced pairing Hamiltonian assumes the form:

\[ H_{\text{pair}} = \sum_k (\epsilon_k - \mu) c_k^\dagger c_k + \sum_{kk'} V_{kk'} c_{k'}^\dagger c_k c_{-k} c_{-k'} \tag{2} \]

where in the tight-binding approximation, \( \epsilon_k = -2t(\cos k_x + \cos k_y); V_{kk'} = V_0(\cos(k_x - k'_x) + \cos(k_y - k'_y)) \), which is non-separable. Using the standard BCS variational ansatz, \( |\Phi_{\text{BCS}}\rangle = \prod_k (u_k + v_k c_k c_k^\dagger)^{\dagger} \), we obtain the \( T = 0 \) gap equations for the gap functions \( \Delta_k^d,s = \Delta_{\alpha}(f)(\cos k_x \pm \cos k_y) \) with \( d_{x^2-y^2} \) and \( s^\pm \) symmetries,

\[ \frac{1}{V_o} = \frac{1}{2M} \sum_{k} \cos k_x (\cos k_x \pm \cos k_y) \frac{E_{k,d,s}}{E_{k,d,s^\pm}}, \tag{3} \]

where \( E_{k,d,s} = ((\epsilon_k - \mu)^2 + \Delta_{\alpha}^2(\cos k_x \pm \cos k_y))^2)^{1/2} \). The Bogoliubov coefficients are given by,

\[ |u_k|^2; \ |v_k|^2 = \frac{1}{2} (1 \pm \frac{\epsilon_k - \mu}{E_{k,d,s^\pm}}). \tag{4} \]

The ratio \( v_k/u_k = -(E_{k,d,s^\pm} - (\epsilon_k - \mu)) / \Delta_{k,d,s^\pm} \). Following Leggett, we adjust \( \mu \) for strong attractions by supplementing the \( T=0 \) gap equation with the number equation:

\[ N = \sum_k (1 - \frac{\epsilon_k - \mu}{E_{k,d,s^\pm}}); \tag{5} \]

This determines the self-consistently readjusted \( \mu \), which is no longer fixed at the Fermi level, and makes the gap equation applicable over the entire range of filling, thereby the BCS and BEC regimes. To allow for strong scattering, the sums are performed over the entire BZ. The natural momentum cut-off afforded by the lattice avoids any possible ultraviolet divergences.

Remarkable differences in features stem in an essential way from differences in gap symmetry. The \( d_{x^2-y^2} \) gap \( \Delta_{\alpha}^d \) vanishes along the lines \( \pm k_x = \pm k_y \) in the 2D BZ, i.e. at four points on the Fermi surface(s), the location of which depends upon filling. The \( s^\pm \) gap \( \Delta_{\alpha}^s \) coincides with the tight-binding \( \Delta_4 \) at exact 1/2-filling, and is nodeless otherwise. Here, \( \mu \leq 0 \), with \( \mu = -4t \) at the bottom of the band. Owing to particle-hole symmetry, it is sufficient to consider \( 0 \leq f \leq 1/2 \). Upon examination of the gap functions and Eqs. (3-5), the following distinctions everywhere become apparent:

(a) For very low fillings \( f \to 0 \), \( \mu \to -4t \), a threshold coupling is required for pairing in the \( d_{x^2-y^2} \) case, while in the \( s^\pm \) case \( \Delta^s \to 0 \) as \( V \to 0 \) due to a weak singularity at \( \mu = -4t \) on the other hand, at 1/2-filling, due to a weak singularity at \( \mu = 0 \) in the \( d_{x^2-y^2} \) case, \( \Delta^d \to 0 \) as \( V \to 0 \). In the \( s^\pm \) case such a singularity is not present and as \( \Delta^s \to 0 \), \( V/4t \to \pi^2/8 \), i.e. a minimum coupling is needed for pairing. In contrast with \( \Delta_{\alpha}^s(V) \), \( \Delta_{\alpha}^d(V) \) changes slope at \( \mu = -4t \), and hence not smooth everywhere (though continuous).

(b) For small \( k \), we have the following limiting behavior: (i) \( \epsilon_k < \mu(= -4t) \): \( |u_k| \to 1, \ |v_k| \to 0 \); this is the strong-coupling BEC limit. Here the ratio \( v_k/u_k \sim \Delta_{\alpha}^d/2|\mu| \sim (k_x^2 - k_y^2)/2|\mu| \), i.e. analytic. (ii) \( \epsilon_k > \mu(= -4t) \): \( |u_k| \to 0, \ |v_k| \to 1 \); this is the weak-
coupling BCS limit. Here $v_k/u_k \rightarrow 1/(k_x-k_y)$, i.e. non-analytic. (iii) $v_k = \mu (= -4t)$: $|u_k| \neq 0, |v_k| \neq 0$, when $E_k \rightarrow 0$. Then $v_k/u_k \sim (k_x-k_y)/(k_x+k_y)$, i.e. intermediate between (i) and (ii). It may be noted that for d-wave, the quasiparticle excitations in the BCS limit (ii) are “gapless” for some values of $k$, while in the BEC limit (i), $E_k \neq 0$, even for gaps with nodes [22].

Self-consistent numerical solutions of Eqs.(3-5) bear out the above features in detail, and also reveal a number of other features. We scale $\mu, V, \Delta$ by hopping parameter, $t$. At a given filling $f$, both $\Delta^d$ and $\Delta^s$ increase with increasing $V$. While for d-wave it is easier to pair electrons at higher fillings, this is not necessarily the case for $s^*$-wave for the weaker couplings $V/4t \leq 1.5$ and small gaps $\Delta^*/2t \leq 0.5$.

In Fig.1 we show $\mu(V)$ for different fillings $f$. At a fixed $f$, in both the d- and $s^*$-wave cases, $\mu$ decreases with increasing coupling $V$, changing less rapidly for progressively larger $f$. However in the $s^*$ case, $\mu(V)$ exhibits a small “bump” for weaker couplings $V/4t \leq 1.5$. The drop in $\mu$ with increasing attraction is significantly more rapid in the uniform s-wave case; see inset in Fig. 1. Crossover to the BEC regime here is signalled by $\mu(V)$ going below the bottom of the band, i.e. crossing the $\mu = -4t$ line. As Fig. 1 shows, for the d-wave case, this develops at both low and high fillings at some minimum value $V_b/4t$ of the coupling. It is interesting to note that as $f \rightarrow 0$, $V_b/4t \rightarrow 1.8$. At exactly 1/2-filling this coupling tends to infinitely large values. For couplings $V > V_b$, the system is conducive to BEC pairing; for $V < V_b$, the system exhibits BCS-like features.

Fig. 2 shows the behavior of the d-wave gaps as a function of coupling $V$ for different values of the chemical potential $\mu$. The $\mu = -4t$ curve represents the locus of $V_b/4t$ for different fillings (see Fig. 1), and demarcates BEC and BCS -pair regimes. To the left is the $\mu > -4t$ region wherein finite gaps of the BCS or intermediate BCS-BEC types exist. On a given constant-$\mu$ curve it may not be possible to have solutions for any arbitrary filling, but only those that satisfy Eqs. (3) and (4) self-consistently. The inset in Fig. 2 shows the corresponding $\Delta^d(V)$ curves for the $s^*$ case. There are interesting differences with the d-wave results in that the boundary ($\mu = -4t$) separating BEC/BCS regimes is not as clear-cut for the weaker couplings $V/4t \leq 1.5$ and the smaller gaps $\Delta/2t \leq 0.5$, however the $\mu < -4t$ region lies to the right of the $\mu = -4t$ curve as in the d-wave case.

Differences in the gap symmetry manifest in a striking manner in the momentum distribution function, $v_k^2$, and the ratio $v_k/u_k$. For d-wave, for a given filling, in the weak-coupling BCS regime ($V < V_b(f, \mu > -4t)$), $v_k^2$ exhibits a peak centered around the zone center (0,0), that becomes progressively narrower with decreasing filling. Then at the crossover point at $V_b(f, \mu = -4t)$, $v_k^2$
is analytic in both regimes. Similar behavior in $F$ for example, it may be possible to decipher the OP symmetry from numerical calculations show (Fig 3c,3d) that for d-wave, in fillings $f$. As observed above in the limiting cases, the quasiparticle density of states, or coherence factors, $u_k v_k + u_k^* v_k^*$. Angle-dependent or transverse ultrasound attenuation, or quasiparticle tunneling at low fillings are possible experiments.

The Fourier transform of $\rho_{\nu}(k_x, k_y)$, namely, $\rho_{\nu}(x, y)$ may provide yet another interesting way to test our results. In the $d$-wave case, in marked contrast with its behavior in the BCS regime, $\rho_{\nu}(x, y)$ is oscillatory in the BEC regime, and exhibits an inhomogenous “checkerboard-type” pattern as shown in Fig 4(a,b). For the chosen parameters of Fig. 3, the contrast ratio of the lowest density to the peak is roughly 50%, being most sensitive to the location of $\mu(V)$. The length scale is of the order of fractions of lattice spacing. $\rho_{\nu}(x, y)$ is fairly uniform in the $s^*$ case in both regimes. Highly sensitive STM may be able to pick up such distinctions.

Much of the phenomena we have discussed are away from exact 1/2-filling, and at relatively strong coupling, where possible effects of spin density wave (SDW) and charge density wave (CDW) instabilities are expected to be suppressed. Addition of a next-nearest-neighbor hopping would also stabilize the paired state, as well as lower the minimum near-neighbor interaction necessary for a bound-state; we have checked this. We have not explored here the issues of collective modes or phase separation. It may be interesting to extend this work to, for example, finite-T, or to explore whether the inhomogenous density that we find bear relationship to the range/strength of the interaction, or to possible phase separation.

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Our findings suggest that experiments, that may be able to directly or indirectly probe $v_k^2$ or combinations of $u_k$ and $v_k$, could reveal novel aspects of the paired states. For example, it may be possible to decipher the OP symmetry (e.g. $d$- or $s^*$-wave) by measuring $v_k^2$ as a function of filling (especially at low-fillings), and/or for different interaction strengths, both of which can be controlled in optical lattices. At the BCS-BEC crossover, we expect the behavior to be quite different depending on whether the OP is $d$- or $s^*$-wave. Also, in the case of $d$-wave pairs, quantities sensitive to $v_k^2$ or to $(u_k, v_k)$ should be very different depending on whether the paired state is BEC or BCS like. A possible probe may be ARPES. Information may also be obtained from experiments that sample the quasiparticle energy $E_k = (\Delta_k^2 + u_k^2)/2$ (related to $u_k, v_k$), the quasiparticle density of states, or coherence factors, $u_k v_k + u_k^* v_k^*$. Angle-dependent or transverse ultrasound attenuation, or quasiparticle tunneling at low fillings are possible experiments.

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