Signatures of Fermion Pairing with Unconventional Symmetry Around the BCS-BEC Crossover in a Quasi-2D Lattice

Dušan Volčko and Khandker F. Quader

Department of Physics, Kent State University, Kent, Ohio 44242, USA

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We consider fermions on a 2D square lattice with a finite-range pairing interaction, and obtain signatures for unconventional pair-symmetry states, $d_{x^2-y^2}$ and extended-s (s^*), in the Bardeen-Cooper-Schrieffer–Bose-Einstein Condensation crossover region. We find that the fermion momentum distribution function, v_k^2, the ratio of the Bogoliubov coefficients, v_k/u_k, and the Fourier transform of v_k^2 are strikingly different for d and s^* symmetries in the crossover region. The chemical potential and the gap functions for both pairing symmetries show several interesting features as a function of interaction. Fermionic atoms in 2D optical lattices may provide a way to test these signatures. We discuss current generation cold atom experiments that may be utilized.

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In recent years, there have been fascinating discoveries of several classes of systems exhibiting many-body states with paired fermions, that may have unconventional pairing symmetry, different from that in the s-wave Bardeen-Cooper-Schrieffer (BCS) case. These range from heavy fermions, high-T_c cuprates, iron-pnictides, to ultracold fermions. There are intense theoretical and experimental efforts aimed at deciphering pairing symmetries or mechanisms in these systems.

Ultracold neutral atoms [1] present an unprecedented opportunity to study the physics of quantum many-particle systems. Subjected to positive and negative detuning using the Feshbach resonance technique, these provide realizations of weak-coupling BCS to strong coupling Bose-Einstein Condensation (BEC) crossover behavior, and the unitarity limit, where the scattering length is infinite.

Cold fermionic atoms in *optical lattices* [2,3] constitute an intriguing set of systems. Tunability of filling (particles per site), hopping kinetic energy or interparticle interaction render optical lattices unprecedented testing grounds for models of correlated electron systems. It has been suggested [4] that atoms in optical lattices, confined to the lowest Bloch band, can be represented by the archetypal condensed matter Hamiltonian, the Hubbard model with hopping t between neighboring sites, and on-site interaction U. Interatomic magnetic or electric dipole interactions, and possibly multiband couplings, can result in finite-range interactions, that could simulate the extended Hubbard model [5]. Duan [6] has shown that on different sides of a broad Feshbach resonance, the effective Hamiltonian can be reduced to a t-J model, familiar in studies of correlated electron systems, J being related to spin or magnetic coupling. Calculations [7–9] predict that attractive-U Hubbard model gives rise to s-wave superconductivity, while the repulsive-U model results in an antiferromagnetic or a d-wave superconducting phase depending on filling. It has been suggested [10] that the underlying physics of the high T_c superconductors may be understood by studying optical lattice systems. Also, due to the possibility that the cuprates, possessing short coherence lengths, could fall in the BEC-BCS crossover region, the crossover problem [11,12] has received considerable theoretical attention. Several authors employed continuum models [7,13–16], focusing mostly on conventional s-wave pair symmetry. Lattice models with on-site or nearest-neighbor attractions have also been considered [7,13,16–18]. There is also a large body of theoretical work [19,20] specific to cold fermions.

Observation of Mott-insulator behavior [21] and s-wave superfluidity (for attractive interactions) [22] in 3D optical lattices represent remarkable feats. Current searches for new phases, such as antiferromagnetism or unconventional pairing, are greatly facilitated by recent development of analogs to existent powerful experimental tools in condensed matter physics. Examples of these new tools are momentum resolved radio frequency (rf) and rf pairing gap spectroscopies [23,24], tomographic rf spectroscopy [25], out of lattice time-of-flight measurements [26], fluorescence imaging [27], and momentum-resolved photoemission spectroscopy [28], analogous to angle-resolved photoemission spectroscopy (ARPES) in condensed matter [29].

In this Letter, we study zero temperature fermion pairing in a 2D square lattice in the BEC-BCS crossover regime using a finite-range *pairing* interaction. 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^*). We present several new results, in particular, specific signatures of states with *unconventional pairing gap* symmetries as one goes between weak and strong coupling regimes. We expect our results to be of relevance to fermionic atoms in 2D optical lattices, and to correlated fermion model systems these would simulate. A key result is the remarkable behavior of the fermion distribution function, v_k^2, (related to momentum distribution, n_k).

For a d-wave pairing gap function, v_k^2 changes *abruptly* from exhibiting 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. Its Fourier transform exhibits a "checkerboard" pattern in real space. By contrast, v_k^2 changes smoothly in the s^*-wave case. We find similar signatures in the ratio of Bogoliubov coefficients v_k/u_k, related to the phase of the superfluid wave function.

Our finite-range pairing interaction is obtained from the extended Hubbard model for two equal species population system on a 2D square lattice:

$$H = \sum_{\langle ij\rangle\sigma}(-tc_{i\sigma}^\dagger + c_{j\sigma} + \text{H.c.}) + U\sum_i n_{i\sigma}n_{i-\sigma} - V\sum_{\langle ij\rangle\sigma\sigma'} n_{i\sigma}n_{j\sigma'} - \mu_o\sum_i n_i, \tag{1}$$

where t is the hopping, μ_o the unrenormalized chemical potential, U the on-site repulsion and V the nearest-neighbor attraction. σ is the "spin" index, which could refer to hyperfine states in optical lattices. In mean-field theory, the Hartree self-energy terms renormalize μ_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 μ. We work with the renormalized μ so as to properly deal with weak and strong couplings, and take $\mu_{J_i}(f) = J_i f$, where $J_i = U, -V$. The filling $f = N/2M$, with N the number of particles, M the number of lattice sites, and the spin degeneracy factor of 2. In correlated electron systems, interactions are mainly Coulombic in origin, and V is typically an order of magnitude down from U. These are scaled by t for a convenient characterization of weak and strong coupling, and to be broadly applicable. In optical lattices, an *effective* Hamiltonian, similar to Eq. (1), could be deduced with V arising from dipolar, or multiband couplings.

On Fourier transforming and retaining interactions between particles with equal and opposite momentum, the reduced *pairing* Hamiltonian assumes the form

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

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 *nonseparable*. Using the standard BCS variational ansatz, $|\Phi_{\text{BCS}}> = \prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}}c_{\mathbf{k}}^\dagger c_{-\mathbf{k}}^\dagger)|0>$, we obtain the $T = 0$ gap equations for the gap functions $\Delta_k^{d,s} = \Delta_o(f)(\cos k_x \pm \cos k_y)$ with $d_{x^2\text{-}y^2}$ $(-)$ and s^* $(+)$ symmetries,

$$\frac{1}{V_o} = \frac{1}{2M}\sum_k^{\text{BZ}}\frac{\cos k_x(\cos k_x \pm \cos k_y)}{E_k^{d,s^*}}, \tag{3}$$

where $E_k^{d,s^*} = [(\epsilon_k - \mu)^2 + \Delta_o^2(\cos k_x \pm \cos k_y)^2]^{1/2}$. The Bogoliubov coefficients are given by

$$|u_{\mathbf{k}}|^2; \qquad |v_{\mathbf{k}}|^2 = \frac{1}{2}\left(1 \pm \frac{\epsilon_k - \mu}{E_k^{d,s^*}}\right). \tag{4}$$

The ratio $v_{\mathbf{k}}/u_{\mathbf{k}} = -[E_k^{d,s^*} - (\epsilon_k - \mu)]/\Delta_k^{d,s^*}$. We readjust μ for strong attractions by supplementing the $T = 0$ gap equation with the number equation [12]

$$N = \sum_k^{\text{BZ}}\left(1 - \frac{\epsilon_k - \mu}{E_k^{d,s^*}}\right). \tag{5}$$

This determines the self-consistently readjusted μ, 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, sums are performed over the entire BZ. The natural momentum cutoff afforded by the lattice avoids any possible ultraviolet divergences.

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

(a) For low fillings ($f \to 0$, $\mu \to -4t$), a threshold coupling is required for d-wave pairing, while in the s^* case, $\Delta^{s^*} \to 0$ as $V \to 0$ due to a weak singularity at $\mu = -4t$. At 1/2 filling, however, due to a weak singularity at $\mu = 0$ in the d-wave case, $\Delta^d \to 0$ as $V \to 0$. For s^*, this singularity is not present, so, as $\Delta^{s^*} \to 0$, $V/4t \to \pi^2/8$, i.e., a minimum coupling is needed for pairing. In contrast with $\Delta_0^{s^*}(V)$, $\Delta_0^d(V)$ changes slope at $\mu = -4t$, and hence not smooth everywhere (though continuous).

(b) For small momenta k, the system exhibits 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 $v_k/u_k \sim \Delta_k/2|\mu| \to (k_x^2 - k_y^2)/2|\mu|$, i.e., *analytic*. (ii) $\epsilon_k > \mu(= -4t)$; $|u_k| \to 0$, $|v_k| \to 1$; this is the weak-coupling BCS limit. Here, $v_k/u_k \to 1/(k_x - k_y)$, i.e., *non-analytic*. (iii) $\epsilon_k = \mu(= -4t)$; $|u_k| \neq 0$, $|v_k| \neq 0$, when $E_k \to 0$. Then $v_k/u_k \sim (k_x - k_y)/(k_x + k_y)$, i.e., intermediate between (i) and (ii). For d waves, 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 [30].

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

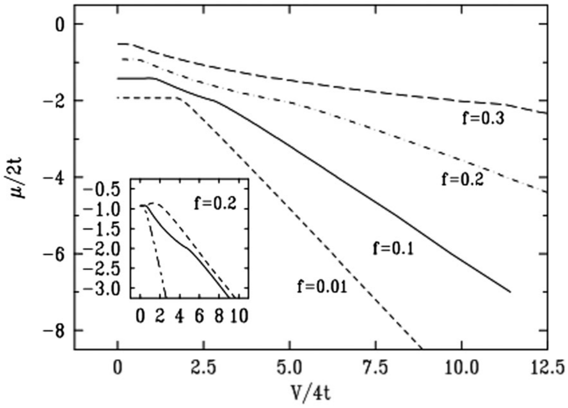

FIG. 1. Chemical potential μ versus coupling V at different fillings f for d-wave pairing. BEC pairs appear where $\mu(V)$ crosses the $\mu/2t = -2$ line. The inset shows $\mu(V)$ for s- (dashed-short dashed line), s^*- (dashed line), and d-wave (solid line) pairing at $f = 0.2$.

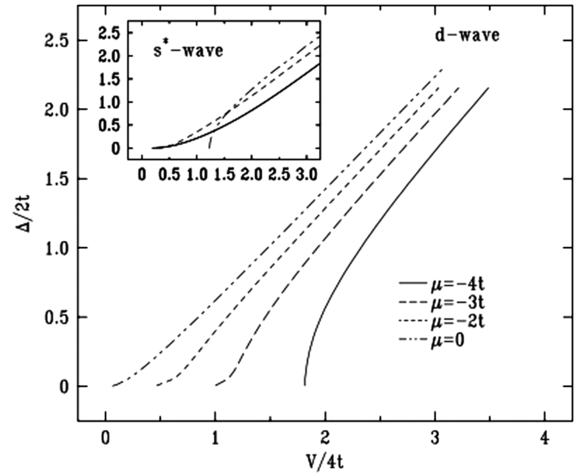

FIG. 2. d-wave gap functions $\Delta/2t$ vs nearest-neighbor coupling $V/4t$ for different chemical potential μ. Inset: Results for the s^* case. $\mu = -4t$ demarcates BEC and BCS regimes.

In Fig. 1 we show $\mu(V)$ for different fillings f. At a fixed f, in both the d- and s^*-wave cases, μ decreases with increasing coupling V, changing less rapidly for progressively larger f. However, as shown in the inset, for s^*-waves, $\mu(V)$ exhibits a small "bump" for weaker couplings $V/4t \leq 1.5$; for the uniform s-wave, the drop in μ with V is significantly more rapid. Crossover to the BEC regime is signaled by $\mu(V)$ going below the $\mu = -4t$ line. As Fig. 1 shows, for d waves, this develops at all fillings for some minimum coupling $V_b/4t$. We note that as $f \rightarrow 0$, $V_b/4t \rightarrow 1.8$; at $1/2$ filling, this coupling tends to infinitely large values. For $V > V_b$, the system is conducive to BEC pairing, and for $V < V_b$, the system exhibits BCS-like features.

Figure 2 shows the behavior of d-wave gaps as a function of coupling V for different values of the chemical potential μ. 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-μ 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 $\Delta^{s^*}(V)$ curves for the s^* case. There are interesting differences with the d-wave results in that the boundary ($\mu = -4t$) separating the BEC-BCS regimes is not as clear cut for weaker couplings $V/4t \leq 1.5$ and 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 waves, 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 narrow with decreasing filling. Then at the crossover point at $V_b(f)$ ($\mu = -4t$), v_k^2 *abruptly* goes to zero around (0, 0), and shows a drastic redistribution along $(0, \pm\pi)$, and $(\pm\pi, 0)$ of BZ. The abruptness is manifested in a "jump" in v_k^2 as the chemical potential goes from just above the bottom of the band ($\mu > -4t$) to just below ($\mu < -4t$), i.e., from BCS to BEC regime. A representative case is shown in Figs. 3(a) and 3(b). In marked contrast, for s^* waves, [Figs. 3(e) and 3(f)], the zone center peak in v_k^2 decreases *smoothly* as one goes from the BCS to the BEC regime; only a slight redistribution occurs at $(\pm\pi, \pm\pi)$. This behavior is replicated at all fillings $f < 1/2$. As noted above, in the small-k limiting cases, our numerical calculations show [Figs. 3(c) and 3(d)] that for d waves, in the weak-coupling BCS regime, v_k/u_k is nonanalytic at $\pm k_x = \pm k_y$; in the strong-coupling BEC regime, v_k/u_k is analytic, vanishing along the zone diagonals and peaking about $(\pm\pi, 0)$ $(0 \pm\pi)$. In the s^* case (not shown), v_k/u_k is analytic in both regimes. Thus we expect states with d- or s^*-pairing gap symmetry to exhibit contrasting behavior at the BCS-BEC crossover, i.e., the unitarity limit.

The Fourier transform of $v_k^2(k_x, k_y)$, namely, $\rho_v(x, y)$ reflects these differences. In the d-wave case, in marked contrast with its behavior in the BCS regime, $\rho_v(x, y)$ is *oscillatory* in the BEC regime, and exhibits an inhomogenous "checkerboard-type" pattern; see Figs. 4(a) and 4(b). For the 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. $\rho_v(x, y)$ is fairly uniform in the s^* case in both regimes.

For correlated electrons, existent experimental techniques can reveal the proposed signatures to distinguish between states with d or extended-s (s^*) symmetry; e.g., v_k^2, its Fourier transform, and quasiparticle energy could be deduced from ARPES [29], pair symmetries from quasiparticle tunneling or scanning tunneling microscopy [31]. In cold fermion systems, v_k^2, and its Fourier transform, could be determined from time-of-flight [26] measurements, in which atoms are released from the lattice, and imaged at a later time. Combined with rf pairing gap

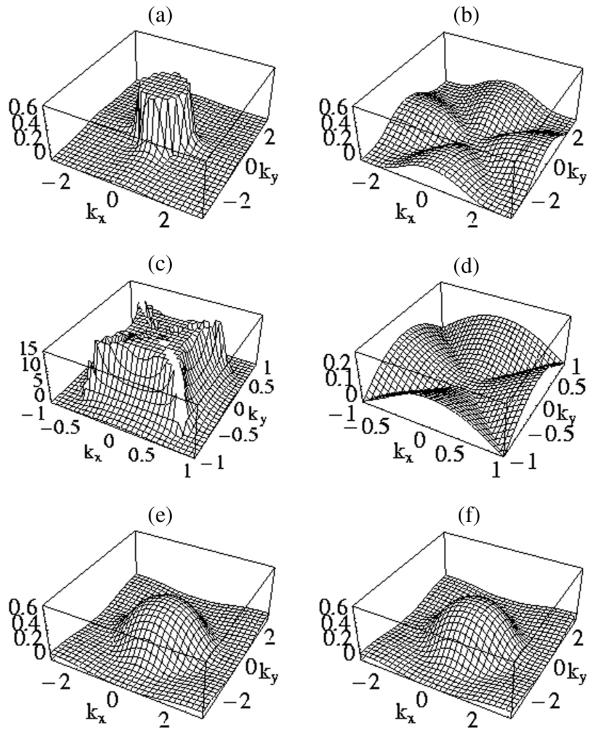

FIG. 3. (a), (b) 3D plots of d-wave fermion distribution functions v_k^2 vs $k_x - k_y$ at filling $f = 0.1$, showing abrupt "jump" in v_k^2. In the BCS regime (a) $\mu = -3t$, $\Delta^d = 5.2t$, $V = 18.7t$, and in the BEC regime (b), $\mu = -6t$, $\Delta^d = 0.6t$, $V = 5.2t$. (c), (d) 3D plots of d waves v_k/u_k vs $k_x - k_y$ for the same parameters as in (a) and (b), respectively. In the BCS regime (c) it can be seen to be nonanalytic; in the BEC regime (d) it is analytic. (e), (f): The same as in (a), (b), but for s^* waves; the behavior is smooth.

spectroscopy [24,32] (analog of tunneling), this could decipher the pairing symmetry. Momentum-resolved rf spectroscopy [23,28], could provide information on the quasiparticle energy $E_k = (\Delta_k^2 + \epsilon_k^2)^{1/2}$, thereby shedding light on (u_k, v_k) and density of states.

Here we have considered a homogeneous Fermi system, so as to appeal broadly to both condensed matter and cold atom physics. While we expect key aspects of our results to hold for cold fermion systems in the presence of atomic traps, we comment on possible effects of the trap. But, first, we note that we consider a pairing Hamiltonian based on

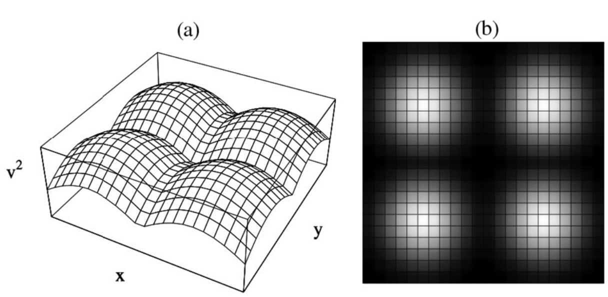

FIG. 4. (a) Fourier transform $\rho_v(x, y)$ of a typical d-wave fermion distribution function, v_k^2. Here, filling $f = 0.01$, $\mu = -4.2t$ (strong-coupling regime), gap $\Delta = .76t$. (b) Projection of (a) to show a contrast ratio of $\rho_v(x, y)$.

the extended Hubbard model, and not the simple Hubbard model, on which most discussions in cold atom literature are based. We are also away from $1/2$ filling, and at relatively strong coupling, so that possible effects of spin density wave and charge density wave instabilities are expected to be suppressed. We have checked [13] that the addition of next-near-neighbor hopping tends to stabilize the paired state, as well as lower the minimum near-neighbor interaction necessary for a bound state.

Away from $1/2$ filling (lower fillings) for a 2D lattice in the presence of a trap [within local density approximation], the multitude of quantum phases obtained [33–35] near $1/2$ filling may not exist [33,34], leaving a metallic state from the trap center to the edge. Thus, for this range of fillings, our results are not expected to be subject to competing signatures from other possible phases in rf spectra. Closer to $1/2$ filling, within local density approximation, there may be other phases, e.g., pairing in different shells behaving as infinite system in each shell [35]. Then, tomographic (spatially resolved) rf spectroscopy [25], using *in situ* phase contrast imaging technique, would be able to probe each shell region, within each of which our results should hold.

Recent work [36] have pointed out possible effects of trap inhomogeneity on the Hartree term, and consequently on rf spectra. In this work, Hartree effect on self-energy is obtained at first-order, so the role of higher-order terms towards a convergent result is not clear at this point. It may also be interesting to examine Hartree effect for the extended Hubbard model on which our calculation is based; this is outside the scope of current work.

Our calculation is at $T = 0$, and any Berezinski-Kosterlitz-Thouless transition [37] would only be revealed in a finite-T calculation. Also, like others, we take our the system to be not strictly 2D, but quasi 2D, with the assumption that a weak link along the third direction stabilizes phase transitions like superfluidity. Our $T = 0$ consideration does not lend itself to calculations of critical temperature, T_c. However, based on other work [10,38], for d-wave pairing we estimate that in electron systems, such as the cuprates, $T_c/T_F \sim 0.015$–0.03, giving a $T_c \sim$ 15–30 K for a $T_F \approx 10^3$ K; in cold fermions, $T_c/T_F \sim 0.01$, giving a $T_c \sim 30$ nK for a $T_F \approx 3$ μK. Thus, for d-wave T_c measurements in cold fermions, realizing temperatures below the currently attainable $T/T_F \simeq 0.05$ is needed. However, these are lower bound estimates, and we expect our proposed signatures to persist to higher temperatures. Recent suggestions [39] of novel cooling methods are encouraging.

Our calculations, in the spirit of BCS and BEC-BCS crossover theories, consider d- and extended-s (s^*-) wave pairing symmetries, independent of pairing mechanisms. Though mean field in nature, we expect the calculated signatures of unconventional pairing symmetries to hold in calculations beyond mean fields. A recent Monte Carlo work [20] on fermions on 2D optical lattice, though at $1/2$ filling, goes beyond mean field and contain substantial discussions regarding possible phases.

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