Superfluid-insulator transitions at non-integer filling in optical lattices of fermionic atoms

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We determine the superfluid transition temperatures $T_c$ and the ground states of the attractive Hubbard model and find new insulating phases associated with non-integer filling at sufficiently strong pairing attraction $|U|$. These states, distinct from band and Mott insulating phases, derive from pair localization; pair hopping at large $|U|$ and high densities is impeded by inter-site, inter-pair repulsive interactions. The best way to detect the breakdown of superfluidity is using fermionic optical lattices which should reveal new forms of “bosonic” order, reflecting ground state pairing without condensation.

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The attractive Hubbard Model has captured the attention of the theoretical and experimental communities, although this model is far from fully understood. It is hoped that experiments using ultracold fermionic atoms in optical lattices will shed light both on competing ground states and on finite temperature $T$ effects, and moreover, provide insights into high temperature superconductivity, largely through the very ubiquitous “pseudogap” effects. These derive from the fact that as the attraction becomes stronger, pairing takes place at a different temperature, $T^*$ from superfluid condensation, $T_c$.

For bosonic systems at half filling the strong (repulsive) interaction limit gives rise to superfluid-Mott insulator transitions. It is a central goal of this paper to investigate this counterpart strong (attractive) interaction regime for fermions and demonstrate that superfluid-insulator (SI) transitions (away from integer filling) are also present. Indeed, the latest experiments on fermions reveal competing insulating and superfluid ground states. It is not yet clear whether these insulating phases are band insulators or localization-induced insulating phases. We note that the largest coupling regime we address in this paper has not yet studied by Monte Carlo (MC) as well as dynamical mean field theoretic approaches. Our work can be contrasted with previous studies, which focused only on $T = 0$ and with Monte Carlo (MC) as well as dynamical mean field theoretic approaches. In the moderate coupling regime, where comparisons can be made, we find transition temperatures to be of comparable order of magnitude, albeit slightly larger (factors of 2). In part this derives from the fact that the standard BCS-Leggett ground state considered here does not include the Gorkov–Melik-Barkhudarov effect. This semi-quantitative difference should not be of concern because different MC calculations of $T_c$ in a unitary Fermi gas have not yet converged to better than factors of 1.5.

Our finite $T$ approach to the Hubbard model includes pair fluctuations in a manner which is consistent with the standard BCS-Leggett ground state and, most importantly, with a proper and physical treatment of pseudogap effects. We stress, however, that these non-condensed pair effects must necessarily be treated differently from previous Nozières–Schmitt-Rink based approaches to $T \neq 0$. Indeed, following Ref. [1], essentially all other pairing fluctuation approaches to BCS-BEC crossover contain an inherent inconsistency; they presume that in the fermionic dispersion relation $E_k = \sqrt{\xi_k^2 + \Delta^2(T)}$, the so-called pairing gap $\Delta$ vanishes at and above $T_c$. These non-condensed pairs (present for all $0 < T < T^*$) are also essential for arriving at physical values for the transition temperature $T_c$. Without including them it is not possible to know about ground states with $T_c \neq 0$, which will naturally occur, e.g., in the present theory in two-dimensional lattices, as compatible with the Mermin-Wagner theorem (in the absence of Kosterlitz-Thouless or other topological order). This underlines the fact that one cannot solve the BCS-Leggett $T = 0$ equations in isolation to characterize the stable ground states.

Our principal result is that, in addition to the expected band insulating state (at filling $n = \frac{1}{2}$), a new insulating phase, which is stabilized by pair fluctuations, emerges when $n$ and the interaction strength exceed appropriate critical values. Strikingly, the critical value for the dimensionless interaction strength is comparable to that found for the Bose Hubbard model [4]. This new insulating phase is different from the Mott or band insulator, both of which occur only at integer filling, but like the Mott case it is due to localization (of fermion pairs). To address cold atom optical lattices, we also extend the attractive Hubbard model to a two-channel model and find that the insulating phases at non-integer filling survive; thus, pair localization is a robust effect.
so restricted that their effective mass diverges prematurely before $|U| \to \infty$. This localization, in turn, is associated with the breakdown of superfluidity.

This frustration of superfluidity at high $n$ can also be addressed via a mapping to a magnetic model. When $|U|/t \gg 1$ the attractive Hubbard model is equivalent to an effective quantum XXZ model with coupling constants $J_{X, Y} = J_{Z}$, both of which are proportional to $t^{2}/|U|$. This mapped problem is subject to the constraint that the average magnetization along the $z$-axis is fixed at $(n - 1)/2$, making this a rather difficult magnetic model to solve in general. Superfluidity corresponds to ordering in the $x - y$ plane. When $n$ is small, the constraint is straightforward to implement and superfluidity emerges. However, at high densities ($n \approx 1$) new states with order along the $z$-axis are expected to emerge, thereby, destroying the superfluid phases. Indeed, it is well known that for $n$ strictly equal to 1, the simple superfluid ground state is undermined as a result of a degeneracy with a charge ordered ground state.

We now address these effects by investigating the physics of fermions which interact via $s$-wave attraction in a three dimensional (3D) square lattice, we start with the one-channel attractive Hubbard model Hamiltonian

$$ H_f = \sum_{k \sigma} \xi_k c^\dagger_{k \sigma} c_{k \sigma} + U \sum_{k \leq q} c^\dagger_{k+q/2} c^\dagger_{-k+q/2} c_{-k+q/2} c_{k+q/2}. $$

Here $\xi_k = \epsilon_k - \mu$, where $\mu$ is the chemical potential. The one-particle energy dispersion is $\epsilon_k = 2t(3 \cos k_x \cos k_y - \cos k_z)$ in a one-band nearest-neighbor tight-binding approximation, where the values of $k$ are restricted in the first Brillouin zone, and we set lattice constant $a_0 = 1$. $U$ represents the attractive on-site coupling. “Resonant” scattering, which corresponds to an infinite two body scattering length, occurs at $U/t \approx -7.915$, in agreement with Ref. [10]. Note that by adopting the Hubbard model we drop any terms associated with direct pair hopping which should not be important in the regime we focus on here where $\mu$ is positive or only slightly negative. We consider a one band model, on the premise that multi-band effects will change the results quantitatively but not qualitatively. There is still uncertainty in the literature [12] about whether or not an effective one band model [9] is adequate.

We use a $T$-matrix formalism [8, 17, 18] to address finite temperature. This particular $T$-matrix approach has a crucial advantage because it leads to physical results for the superfluid density $n_s(T)$. This single valued, monotonic and continuous behavior (from zero to $T_c$) for $n_s(T)$ is not found in other theories; this physical behavior can be traced to a self consistent treatment of pseudogap effects [3], in which pair fluctuations enter into both the gap and the number equations in a fully self-consistent fashion.

Details of this formalism can be found in [3]. We define the noncondensed pair propagator as $t_{pq}(Q) = U/[1 + U \chi(Q)]$, where, as in Ref. [19], our choice for the pair susceptibility, given by $\chi(Q) = \sum_K G_{0}(Q - K) G(K)$, can be derived from decoupling the Green’s function equations of motion. Here $G(K)$ and $G_{0}(K) = i \omega_n - \xi_k$ are the full and bare Green’s functions. $K \equiv (i \omega_n, k)$ and $Q \equiv (i \Omega_m, q)$ are four-vectors with $\sum_{K} = T \sum_{n} \sum_{k}$. Below $T_c$, the self-energy $\Sigma(K) = \sum_{Q} t(Q) G_{0}(Q - K)$ can be well approximated by the BCS form, $\Sigma(K) = -\Delta^2 G_{0}(-K)$, where $t(Q) = -\langle \Delta_{sc}^{2}/T \rangle \delta(Q) + t_{pq}(Q)$, and $\Delta_{sc}$ is the superfluid order parameter. In the superfluid state, the “gap equation” is given by the pairing instability condition $t_{pq}(0) = U^{-1} + \chi(0) = 0$, which is equivalent to the BCS condition on the pairs. Therefore, we have

$$ \frac{1}{U} = -\sum_{k} \left[ 1 - 2f(E_k) \right]. $$

Here $f(x)$ is the Fermi distribution function. Similarly, the average density $n$ in a lattice, derived from $n = \sum_{K,i} G_{\sigma}(K)$, is given by

$$ n = \sum_{k} \left[ \left( 1 - \frac{\xi_{k}}{E_{k}} \right) + 2f(E_{k}) \left( \frac{\xi_{k}}{E_{k}} \right) \right]. $$

We next determine the dispersion relation and the number density for noncondensed pairs. From the self-energy expression one obtains $\Delta_{pg}^{2} = \Delta_{sc}^{2} + \Delta_{pg}^{2}$ where the pseudogap contribution satisfies [3, 18, 19]

$$ \Delta_{pg}^{2} \equiv -\sum_{Q} t_{pq}(Q), $$

which can be shown to vanish at $T = 0$. The critical temperature $T_c$ is defined as the lowest temperature where $\Delta_{sc} = 0$. In the superfluid phase (pair chemical potential $\mu_{pair} = 0$), and at small $Q$, $t_{pq}(Q) = \chi(Q) - \chi(0) \approx Z_{1} \Omega^{2} + |Z_{0}| \Omega - \xi^{2} q^{2}$. Except when particle-hole symmetry is present, e.g., at very weak coupling and near half filling, we find $Z_{1} \ll |Z_{0}|$, which thus is irrelevant. Near $n = 1$, the $Z_{1} \Omega^{2}$ term enters and regularizes the van Hove singularity. To first order in $\Omega$ one can write $\Delta_{pg}^{2} = |Z_{0}|^{-1} \sum_{Q} b(Q)$, where $b(x)$ is the Bose distribution function. At sufficiently low $q$, we can approximate the dispersion of the noncondensed pairs by $\Omega_{eq} = q^{2}/2M^{*}$, where $M^{*}$ is the effective mass of pairs at the bottom of the band.

In Fig. we show $T_c/E_F$ as a function of $U/t$ for several values of $n$ in the one-channel model. Here $E_F$ is the Fermi energy of a non-interacting Fermi gas with the same filling factor. As in MC simulations, $T_c$ exhibits a maximum near resonance and decreases slightly when $U/t$ is away from resonance. When $n$ is small, we find a long tail in $T_c$ proportional to $t^{2}/|U|$, as expected [7]. Importantly, it is observed that when $n > n_c \approx 0.53$, $T_c$ vanishes provided $U/t$ exceeds a critical value $(U/t)_{c}$. It should be noted that at the insulating onset point, we find $\mu$ is zero or slightly positive, far from the true bosonic regime. The inclusion of pair fluctuation effects is essential here for establishing $T_c = 0$ beyond $(U/t)_{c}$. This result can be contrasted with the predicted ground state of strict mean-field theory shown in the inset of Fig where $\Delta/\lambda$ vanishes only at $n = 0$ and $n = 2$ (band insulator).

In Fig. we show typical phase diagrams at low and high densities. In contrast to $T_c$, the pairing onset temperature $T^{*}$
is marked next to each curve. The vertical dashed line indicates the
unitary limit. Inset: \( T = 0 \) mean-field results for \( \Delta / t \) as a function of
\( n \).

![Figure 1](image1)

**Figure 1:** \( T_c / E_F \) as a function of \( U / t \). The corresponding value of
\( n \) is marked next to each curve. The vertical dashed line indicates the
unitary limit. Inset: \( T = 0 \) mean-field results for \( \Delta / t \) as a function of
\( n \).

![Figure 2](image2)

**Figure 2:** Phase diagrams of one-channel attractive Hubbard model
at (a) \( n = 0.3 \) and (b) \( n = 0.7 \). 'SF' denotes superfluid, 'PG'
denotes pseudogap phase and 'Insulator' in (b) schematically indi-
cates breakdown of ground state superfluidity. Inset: \( T = 0 \) phase
diagram. Here the boundary separating BCS and BEC regimes is de-
termined when \( \mu \) reaches the bottom of the band. The gray shaded
area shows where superfluid does not exist, corresponding to the 'Ins-
ulator' regime.

(As estimated from the strict mean-field solution for \( T_c \)), in-
creases monotonically with \( |U| / t \). The high density phase di-
agram, in particular, bears some similarity to its counterpart
in high temperature superconductors [5]. In both figures, as in
high \( T_c \) superconductors, we see an anti-correlation between
the behavior of \( T_c \) and \( T^* \), associated with lattice [1] as well
as pseudogap effects [8]. The complete suppression of su-
perfluidity in Fig. 2(b) can be shown explicitly to come from
localization of pairs; that is, the effective pairwise mass \( M^* \to \infty \).

In the inset of Fig. 2 we show the \( T = 0 \) phase diagram,
in which “BCS” (“BEC”) denote states with \( \mu \) higher (lower)
below the bottom of the band. The shaded regime corresponds
to where there is a non-superfluid ground state. The lowest value of
\( \langle |U| / t \rangle \approx 25 \) occurs at \( n = 0.53 \). This is com-
parable in magnitude to the critical value \( |U| / t \approx 35 \) of the
Mott-superfluid transition of the 3D boson (reptile) Hu-
bard model with filling factor \( 1 \) [4], although the physical ori-
gin of the two insulators is different.

In actual experiments, attractive interactions between the
atoms are generated by Feshbach resonance effects, which
in principle, require a two-channel description. Previous
work on the two-channel model in a lattice concentrated
on the superfluid-Mott transition in the strongly-interacting
regime near \( n = 2 \) [10, 11]. Other recent work dis-
cussed band insulators in the weakly-interacting regime [12].
The generalization of our \( T \)-matrix formalism to the two-
channel model for Fermi gases was presented in [13]. To
take into account the closed-channel molecules, the Hamil-
tonian is extended to \( H = H_f + H_b + H_{fb} \), where
\( H_b = - \sum_{\mathbf{q}} \epsilon_{\mathbf{q}}^b b_{\mathbf{q}}^\dagger b_{\mathbf{q}} \) describes the hopping of molecules and
\( H_{fb} = \sum_{\mathbf{q}, \mathbf{k}} g(b_{\mathbf{q}}^\dagger c_{\mathbf{q}+\mathbf{k}} + \text{h.c.}) \) describes
conversion between molecules and fermion pairs. Here \( \epsilon_{\mathbf{q}}^m =
\epsilon_{\mathbf{q}}^b - 2\mu + \nu \), \( \nu \) is the magnetic detuning, and \( g \) is the coupling
constant for molecule-pair conversion. The strength of the at-
tractive pairing interaction is modified relative to the one band
case [18] to

\[
U_{\text{eff}}(Q) = U + g^2 D_0(Q)
\]

where \( D_0(\mathbf{Q}) = 1/(\Omega_n - E_{\mathbf{Q}}^m) \) is the propagator for non-
interacting closed channel molecules. The gap equation in-
volves only \( U_{\text{eff}} \equiv U_{\text{eff}}(Q = 0) \). The density in the lattice
now becomes \( n = n_f + 2n_h + 2n_{\mathbf{Q}} \) where the open-channel
contribution \( n_f \) is given by Eq. (3) and the closed-channel
contribution comes from the molecular condensate \( 2n_{\mathbf{Q}} \), and
non-condensed molecules \( 2n_h \). The energy dispersion of
molecules has a Bloch-like dispersion, just as found for the
fermions. In the long wavelength limit, we may expand this
Bloch band dispersion as \( \epsilon_{\mathbf{Q}}^m \approx q^2/2M_h \), where \( M_h = 2/t \)
is the effective bare mass of the molecules. The fermion pairs
have a similar \( q^2 \) dispersion and, in general, hybridize strongly
with these closed-channel molecules.

In our Hamiltonian we have dropped a direct closed-
channel boson-boson repulsion. This was included in previous
work [10, 11] which aimed to create Mott insulating phases
associated with the closed channel. At \( n = 2 \), because the
closed channel represents a band which is never completely
filled (due to the presence of the open channel), we find that
localized states in the strict Mott sense are not obtainable as is
consistent with Ref. [11]. In this way we argue that it is appro-
priate here to drop the intra-closed-channel interactions. We
note parenthetically that to obtain a Mott insulating state one
possibility is to treat the closed channel as composite fermion
pairs (or hard-core bosons [11]) and to consider filling above
\( n = 2 \).

Figure 3 shows \( T_c / E_F \) in the two-channel model as a func-
tion of \( U_{\text{eff}}/t \) for [(a) and (c)] narrow and (b) broad Fes-
bach resonances. Here \( U_{\text{eff}} \) is tuned via \( \nu \) with fixed \( U \)
and \( g \) in (a) and (b) and via \( U \) with fixed \( \nu \) and \( g \) in (c).
Figure 3(a) corresponds to the case in which there is a con-
siderable admixture of both closed and open channels. We
take \( U/t = -6 \) and consider a relatively narrow resonance,
\( g/t = -60 \), as well as two values of \( n = 0.7 \) and \( n = 2 \). For
\( n = 0.7 \), \( T_c \) is first suppressed by the opening of the pseudo-
gap as \( -U_{\text{eff}} \) increases; then \( T_c \) eventually increases with in-
creasing \(-U_{\text{eff}}\) as fermions are converted into closed-channel
molecules which have a finite BEC transition temperature. For
Figure 3: $T_c/E_F$ as a function of pairing interaction $U_{\text{eff}}/t$ in the two-channel model, as tuned by (a) detuning $\nu$ and (c) $U$ for relatively (a,c) narrow and (b) broad Feshbach resonances. There parameters are: (a) $g/t = -60, U/t = -6, \nu = 0.7$ (black) and 2 (red curve); (b) $n = 0.7, g/t = -600, U/t = -6$; (c) $n = 0.7, g/t = -60, \nu/t = 500$. The shaded regimes in (b) and (c) schematically indicate the new, non-integer-filling insulating states.

$n = 2$, the cusp in the $T_c$ curve comes from the van Hove singularity at $n_f = 1$. For a large range of $U_{\text{eff}}, T_c$, for $n = 2$ is effectively zero [21], until a sufficient number of open channel pairs are converted to closed-channel molecules. Importantly, for this case, the insulating state thereby observed is a band insulator.

When we decrease the participation of closed channel molecules by either increasing $-U/t$ or $|g|/t$, insulating states (of the new form, at non-integer filling) start to emerge. In Fig. 3(b) we demonstrate these insulating states by plotting $T_c/E_F$ for $n = 0.7$ at $U/t = -6$ and a large $|g|/t = 600$ (wide resonance) as a function of $U_{\text{eff}}/t$ by tuning $\nu$. In Fig. 3(c) we plot the counterpart curve for a narrower resonance ($g/t = -60$) as a function of $U_{\text{eff}}/t$ by tuning $U$ at fixed high detuning $\nu$. In contrast to the result shown in Fig. 3(a), by decreasing the fraction of closed channel states, as in panels (b) and (c), we find localized insulating phases. This localization can be demonstrated by a divergence in the effective pair mass. In summary, insulating states at non-integer filling are robust even in the presence of closed-channel molecules.

The experimental implications of our work are readily testable, since, fortunately, using Feshbach resonances, current cold atom experiments [2] are able to simulate these attractive Hubbard Hamiltonians. Our principal result is the theoretical observation of superfluid-insulator transitions in the ground state of the attractive Hubbard model away from integer filling. To observe these new phases experimentally one needs to consider average densities $n \approx 1$ and sufficiently large $|U_f|/t$ of the order of, or larger than, that required for superfluid-Mott insulator transitions in Bose gases [4]. Because experimentally there is an additional background harmonic trapping potential, $n$ can never be precisely specified throughout the lattice [20] and thus it should be possible to find extended regions with non-integer filling factors. The tunable parameters in optical lattice experiments are scattering length and lattice potential $V_0$. While it is relatively easy to express $t$ in terms of $V_0$, the conversion of the on-site attraction $U$ in terms of the scattering length and $V_0$ near unitarity is not as straightforward as that in free space [4].

It is clear that the crucial test of the new phase diagram in Fig. 2(b) does not lie in distinguishing whether $T_c$ is small or strictly zero. Rather with $T_c = 0$ one can invoke entropic considerations and deduce that signatures of this new ground state will involve detecting some new form of (bosonic) order. This may be the analogue of a (pair density wave) phase which appears to be present in high temperature superconductors, in the underdoped side of the phase diagram [22].

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