Mott Criticality and Pseudogap in Bose-Fermi Mixtures

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We study the Mott transition of a mixed Bose-Fermi system of ultracold atoms in an optical lattice, where the number of (spinless) fermions and bosons adds up to one atom per lattice, $n_F + n_B = 1$. For weak interactions, a Fermi surface coexists with a Bose-Einstein condensate while for strong interaction the system is incompressible but still characterized by a Fermi surface of composite fermions. At the critical point, the spectral function of the fermions $A(\mathbf{k}, \omega)$ exhibits a pseudogapped behavior, rising as $|\omega|$ at the Fermi momentum, while in the Mott phase it is fully gapped. Taking into account the interaction between the critical modes leads at very low temperatures either to p-wave pairing or the transition is driven weakly first order. The same mechanism should also be important in antiferromagnetic metals with a small Fermi surface.

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A recent experiment with an ultracold mixture of bosonic and fermionic Yb atoms in an optical lattice [1] has found a remarkable quantum phase that can be described as a mixed Mott insulator. Such a state [2–4] is established in the strongly interacting regime when the average site occupation of the bosons and fermions together is an integer, $n_B + n_F = 0, 1, \ldots$. While the state is incompressible and hence fluctuations of the total density are gapped, the fermions can still move around by exchanging with the spinless bosons. Hence, the mobile objects are bound states of a fermionic atom and a bosonic hole. Depending on their effective interactions, these bound states can form a number of different phases, including a Fermi liquid or a paired condensate. But those are rather strange fluids, made of composite fermions that carry zero net particle number. Accordingly, the spectral function of the original fermionic atoms will not display a quasiparticle peak. This phase, established for sufficiently strong interactions, should be contrasted with the weakly interacting limit where the fermionic atoms form a conventional Fermi sea coexisting with a Bose condensate (BEC) of the other species. In this Letter, we investigate the quantum phase transition from the incompressible mixed Mott state to the compressible metal-BEC phase and the fate of the Fermi surface across the transition.

In most solids the Mott quantum critical point (QCP) from a metal to an insulating state is masked by antiferromagnetism. In cases where frustration suppresses magnetism, however, it has been argued that a direct transition from a metallic phase to an insulating and incompressible $U(1)$ spin liquid is possible [5–8]. Yet the understanding of this transition remains rudimentary and is unconfirmed by experiment. We argue that with ultracold mixtures of bosons and fermions it is possible to study a similar transition directly. Although coupling to a deconfined $U(1)$ gauge field is missing in our case, important features, such as critical vanishing of quasiparticle weight and opening of a pseudogap, remain.

Model.—For simplicity, we confine ourselves to spinless fermions mixed with a single species of bosons in three dimensions ($d = 3$), described by the generalized Hubbard model

$$H = -t_b \sum_{\langle ij\rangle} (b_i^\dagger b_j + \text{H.c.}) - t_f \sum_{\langle ig\rangle} (f_i^\dagger f_j + \text{H.c.}) + \frac{1}{2} U_{bb} \sum_i n_{bi}(n_{bi} - 1) + U_{bf} \sum_i n_{bi} n_{fi}. \quad (1)$$

Here $b_i^\dagger$ and $f_i^\dagger$ create bosonic and fermionic atoms, respectively, and n_{bi} (n_{fi}) are the bosonic (fermionic) site occupations. Mott phases can occur for commensurate filling (we take $\langle n_{bi}\rangle + \langle n_{fi}\rangle = 1$).

When the interactions are large enough, $U_{bf} \gg t_f, t_b$ and $U_{bb} \gg t_b$, fluctuations of the density are strongly suppressed and the system is deep in the Mott phase. After eliminating perturbatively the empty and doubly occupied states, one obtains a purely fermionic model [2]

$$H = -t_{\text{eff}} \sum_{\langle ij\rangle} (c_i^\dagger c_j + \text{H.c.}) + V_{\text{eff}} \sum_{\langle ij\rangle} n_i n_j, \quad (2)$$

with $t_{\text{eff}} = t_f t_b / U_{bf}$ and $V_{\text{eff}} = (t_b^2 + t_f^2)/U_{bf} - 2t_b^2/U_{bb}$. Here $c_i^\dagger = f_i^\dagger b_i$ is a composite fermion, quadratic in the original fields, $n_i = c_i^\dagger c_i$ and the vacuum $|\Omega\rangle$ of the composite fermion is the singly occupied bosonic site.

The ground state of the fermion model (2) can be a Fermi liquid for $V_{\text{eff}} \geq 0$, a p-wave superfluid for small or moderately large negative V_{eff}, or be unstable to phase separation for large negative V_{eff}, $|V_{\text{eff}}| \gg t_{\text{eff}}$. A phase transition out of the Mott state is driven by reducing the strength of the interactions U_{bb}, U_{bf}, or both.

Consider first tuning the transition by changing U_{bf}, while U_{bb} remains large. For the resulting hard-core bosons it is useful to rewrite the problem in terms of holes in the Mott insulator, $h_i^\dagger = b_i$. The condition of unity filling reads now $\langle n_{hi}\rangle = \langle n_{fi}\rangle$ and the repulsive interaction is mapped to attraction, $U_{bf} \to -U_{bf}$. In these variables, the Mott transition can be understood as binding of bosons to fermions, with the Mott state being a Fermi liquid of the molecules $c_i^\dagger|\Omega\rangle = f_i^\dagger h_i^\dagger|\Omega\rangle$ as $V_{\rm eff} > 0$ in this limit.

A similar transition, from a Fermi surface of atoms to a Fermi surface of molecules, has been considered in Ref. [9] for a Bose-Fermi mixture in the continuum with an interspecies Feshbach resonance. Our lattice model with $U_{bb} \gg U_{bf}$ maps to this continuum problem for low densities, $\langle n_{fi}\rangle \ll 1$. We therefore expect two transitions as found in Ref. [9]. First a Fermi sea of molecules starts to form beyond a critical value of the attraction $U_{bf} = U_{c1}$ and coexists with the atomic Fermi sea and a BEC. The volume of the molecular Fermi surface grows continuously until it reaches the full Luttinger volume, corresponding to the full fermion density, at $U_{bf} = U_{c2}$, where the condensate fraction vanishes and the Mott insulating state is reached. As pointed out in Ref. [9], interactions are irrelevant at such a QCP in $d = 3$ and due to the quadratic dispersion at the bottom of the bosonic and fermionic bands, $\omega \propto k^2$, the dynamical critical exponent is $z = 2$. The same theory can be applied for nearly unity filling by the fermions if we apply the particle hole transformation on the fermions rather than the bosons. Other phases with broken lattice symmetry are possible at certain intermediate fillings [10,11].

We now turn to the main focus of this Letter and consider the transition driven by reducing the boson-boson interaction U_{bb} for large U_{bf}. In this case we can eliminate the fermionic doublon state $f_i^\dagger b_i^\dagger|0\rangle$. Using again the single boson state $|\Omega\rangle$ as vacuum, we introduce besides the single fermion state $c_i^\dagger|\Omega\rangle$ and bosonic hole $h_i^\dagger|\Omega\rangle$ defined above also the bosonic doublon $p_i^\dagger|\Omega\rangle = 2^{-1/2}b_i^\dagger|\Omega\rangle$. The Hamiltonian (1) projected to low energies becomes

$$\begin{aligned} H_{\rm eff} = {}& \frac{1}{2}U_{bb}\sum_i(n_{pi} + n_{hi}) - \mu_f\sum_i n_{ci} \\ & - t_b\sum_{\langle ij\rangle}[(\sqrt{2}p_i^\dagger + h_i)(\sqrt{2}p_j + h_i^\dagger) + \text{H.c.}] \\ & - t_f\sum_{\langle ij\rangle}(c_i^\dagger h_i h_j^\dagger c_j + \text{H.c}) + U_{cc}\sum_{\langle ij\rangle}n_{ci}n_{cj} \end{aligned} \quad (3)$$

supplemented with the hard-core condition $n_{pi} + n_{hi} + n_{ci} \le 1$ and $U_{cc} = (t_b^2 + t_f^2)/U_{bf}$. Unity filling implies $\langle n_{hi}\rangle = \langle n_{pi}\rangle$ and the transition from the Bose-Fermi Mott state to the superfluid is a simultaneous condensation of doublons and holes just as in a conventional bosonic Mott-superfluid transition [12].

Critical theory.—The most general action (including the most relevant terms) describing the QCP is given by

$$\begin{aligned} S &= S_b + S_f + S_{bf}, \\ S_b &= \int dx d\tau |\partial_\tau\phi|^2 + v_s^2|\nabla\phi|^2 + r|\phi|^2 + u_b|\phi|^4, \\ S_f &= \int \bar\psi[\partial_\tau + \vec{v}_F\cdot(-i\nabla - \vec{k}_F)]\psi - u_f\bar\psi\nabla\bar\psi\cdot\psi\nabla\psi, \\ S_{bf} &= u_{bf}\int dx d\tau \bar\psi\psi|\phi|^2. \end{aligned} \quad (4)$$

Here the bosonic order parameter field is related to the bosons through $\phi(x) \sim \sqrt{1/v_s}[h(x) + p^\dagger(x)]$. As in the conventional bosonic Mott transition, $\langle n_{hi}\rangle = \langle n_{pi}\rangle$ entails the absence of linear time derivatives $\phi^*\partial_\tau\phi$. Formally, the same theory was considered by Yang [13] to address the Mott transition at integer *boson* filling in contact with a Fermi sea at a *noncommensurate* filling. The crucial difference here is that in our theory the ψ fermions are not the physical atoms but rather composite objects. In the Supplemental Material [14] we discuss how the parameters v_s, v_F, u_f, and u_{bf} in Eq. (4) are related to the original coupling constants.

The bosonic sector of the field theory (4) is identical to that of the commensurate Mott transition in the purely bosonic system where $\omega \sim v_s k$, resulting in dynamical exponent $z = 1$. First, we analyze the coupling of the bosons to the fermions by a scaling analysis ($\vec{r} \to \lambda\vec{r}$, $\tau \to \lambda\tau$, $\phi \to \phi/\lambda$, and $\psi \to \psi/\lambda^{3/2}$ in $d = 3$) around this fixed point ($u_f = 0 = u_{bf} = 0$) which shows that u_{bf} is irrelevant, $u_{bf} \to u_{bf}/\lambda$. An alternative scaling scheme [15], leading to the same conclusion is discussed in the Supplemental Material [14]. Moreover, assuming $t_f \ll t_b$, the bare couplings u_f and u_{bf} are small (see Supplemental Material [14]). This does, however, not imply that u_{bf} can be set to zero as upon integrating out the fermions it generates a marginal long-ranged interaction of ϕ, see below. u_f is marginal and leads for $u_f > 0$ to p-wave superfluidity.

We first assume that the pairing instability of the Fermi surface can be neglected as either u_f is repulsive or so small that the transition temperature is smaller than T. Because of the irrelevance of u_{bf} one can integrate out the fermions perturbatively to obtain a purely bosonic theory with a modified quartic interaction term

$$S_{\rm int} = \int[u_0 + u_1 f(\omega/v_F q)]\phi^*_{k-q,\nu-\omega}\phi^*_{k'+q,\nu'+\omega}\phi_{k',\nu'}\phi_{k,\nu}. \quad (5)$$

The ω and q dependence of the new interaction vertex

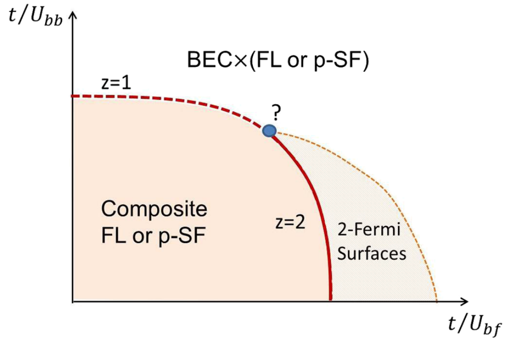

FIG. 1 (color online). Schematic phase diagram of the Bose Fermi mixture at combined integer filling. At weak interaction the bosons form a BEC and the fermions form a Fermi liquid, unstable at very low temperature to p-wave pairing. At strong interactions the system goes into the mixed Mott phase, in which composite neutral fermions (with respect to total density) still exist as low energy degrees of freedom. Depending on parameters they can form either a Fermi liquid (FL), a p-wave superfluid, or phase separate. The nature of the Mott critical point depends on how it is approached, by tuning the boson-fermion or the boson-boson interactions.

$$f(x) = \frac{ix}{2}\ln\left(\frac{ix+1}{ix-1}\right) \tag{6}$$

is inherited from the fermionic density-density correlation function. We obtain $u_1 \approx u_{bf}^2 \nu(0) = 64 v_s^2 v_F = \frac{4}{\pi}\frac{v_F}{v_s} u_b$, where $\nu(0)$ is the fermion density of states. The local interaction u_0 also receives a correction, $u_0 \approx u_b + u_1$.

To investigate the fate of the critical point we set up a perturbative renormalization group (RG) by integrating out momenta with $\Lambda e^{-l} < |q| < \Lambda$. A rescaling, $k \to k e^{-l}$ and $\omega \to \omega e^{-zl}$, restores the original cutoff Λ. Because of the ω dependence of the interactions, already to one-loop order one obtains self-energy corrections which are absorbed by rescaling of the field ϕ and a correction to the dynamical critical exponent z (see Supplemental Material [14]). A complication is that higher-order long range terms of the form $u_n f(\omega/v_f q)^n$ are generated during the RG flow. The scaling is therefore determined by coupled equations for the dimensionless coupling constants $g_n(l) = u_n(l)/(8\pi^2 v_s^3)$ and the dimensionless Fermi velocity $\eta(l) = v_F(l)/v_s$.

$$\frac{d\eta}{dl} = \frac{2}{3}\sum_{m=1}^{\infty} f_m^{\eta}(\eta) g_m,$$

$$\frac{dg_0}{dl} = -10 g_0^2 - 12 g_0 \sum_m f_m^g(\eta) g_m - 4\sum_{m,n=1}^{\infty} f_{m+n}^g(\eta) g_m g_n,$$

$$\frac{dg_n}{dl} = -2\sum_{m=0}^{n} g_{n-m} g_m - 4 g_n \sum_{m=0}^{\infty} f_m^g(\eta) g_m, \quad n > 0, \tag{7}$$

where $f_m^{\eta}(\eta) = \frac{4\eta}{\pi}\int_0^{\infty} \frac{3\eta^2 x^2 - 1}{(\eta^2 x^2 + 1)^3} f(x)^m dx$ and $f_m^g(\eta) = \frac{4\eta}{\pi}\int_0^{\infty} \frac{1}{(\eta^2 x^2 + 1)^2} f(x)^m dx$ are functions of $\eta(l)$.

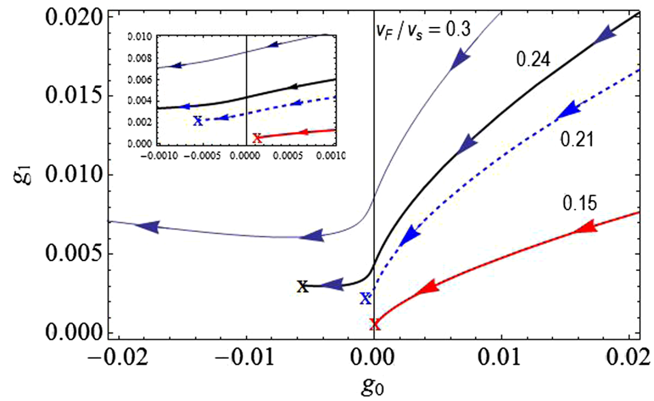

FIG. 2 (color online). RG flow for three different values of the bare Fermi velocity v_F/v_s using $n_{\max} = 13$ (see text). The inset is a zoom near $g_0 = 0$ showing that for the three larger values of v_F/v_s the local interaction is driven to negative values before the flow is cut off at the scale of the pairing gap $\Delta = \epsilon_F \exp(-8\pi v_s/v_F)$. For these values we expect a fluctuation driven first order transition.

In solving for the flow we keep terms with $n < n_{\max}$ and find that the resulting flow converges with $n_{\max}$ (keeping 10–15 terms is enough in practice, see Supplemental Material [14]). This scheme works well since the newly generated interactions are all irrelevant. In two dimensions, where they are relevant the proliferation of terms can be avoided by introducing an auxiliary field [16].

Typical RG trajectories in the subspace g_1 versus g_0 are shown in Fig. 2. Initially, both g_0 and g_1 drop but the flow of g_1 is much slower due to its nonlocal nature. Therefore g_1 is finite when g_0 reaches zero, driving g_0 to negative values through the last term in the flow Eq. (8) for g_0. This leads to a first-order transition.

In the RG approach described above we have neglected the induced attraction u_f between fermions, which would lead to a pairing instability and opening of a gap $\Delta \approx E_F \exp(-8\pi v_s/v_F)$ in the Fermi surface. Such a gap suppresses the nonlocal couplings at low energies $v_s \Lambda e^{-l} < \Delta$. Therefore, if the coupling constants g_n have not yet driven the local coupling g_0 negative at that scale, the first order transition will be avoided. Numerical solution of the flow equations suggest that this is the case if the bare ratio $v_F/v_s < 0.18$, while for $v_F/v_s > 0.18$ we expect a first order transition. In either case the Fermi surface is expected to give way to a small p-wave gap near the transition for $T \to 0$.

Our analysis applies to a number of other QCPs where bosonic and fermionic degrees of freedom coexist. Consider, for example, a metallic commensurate antiferromagnet, where the shape of the Fermi surface is such that the ordering wave vector $\vec{Q}$ does not connect different parts of the Fermi surface. In such a situation only a quadratic coupling of fermions to a $z = 1$ bosonic QCP survives. Our analysis shows that in $d = 3$ this coupling will render the

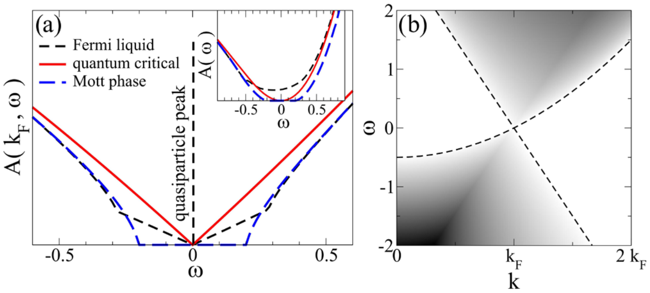

FIG. 3 (color online). (a) Spectral function $A(k, \omega)$ of the fermions at $k = k_F$ in the superfluid phase, critical point, and Mott insulator ($r = -0.04$, 0, 0.04, $v_s/v_F = 3$). Inset: local density of states $A(\omega) = \int dk A(k, \omega)$ in the three cases. (b) The spectral function $A(k, \omega)$ at the critical point.

QCP always weakly first order as long as no superconductivity gaps out the Fermi surface.

Pseudogap.—We now discuss the experimental ramifications of the quantum phase transition focusing on the spectral function associated with emission of a fermionic atom in rf spectroscopy [17,18]. The crucial point is that in the long-wavelength limit the physical atomic fermions f_i are composite objects in terms of the weakly coupled fields ψ and ϕ, $f(x) \sim \sqrt{1/v_s}\phi(x)\psi(x)$ as $f_i = h_i^\dagger c_i$. Hence, the spectral function should be found from the Green's function $\mathcal{G}(x, \tau) = \langle \bar{\psi}(x, \tau)\phi^*(x, \tau)\phi(0)\psi(0)\rangle$.

For the sake of this discussion, we ignore all logarithmic corrections which ultimately lead either to p-wave pairing or the fluctuation induced first order transition. These subtle effects are noticeable only at exponentially low energies. The salient features of the spectral function at higher energies (or temperatures) are captured within the Gaussian theory obtained from expansion about the saddle point of Eq. (4), which implies $\mathcal{G}(x, \tau) = G_\psi(x, \tau)\mathcal{D}_\phi(x, \tau)$, where G_ψ is the free fermion Green's function of the composite fermions.

In the superfluid side, we can take a Bogoliubov expansion of the order parameter $\phi = \phi_0 + \delta\phi_1 + i\delta\phi_2$, to split the bosonic component of the Green's function into three contributions: $\mathcal{D}_\phi(x, \tau) = |\phi_0|^2 + \mathcal{D}_1(x, \tau) + \mathcal{D}_2(x, \tau)$. The condensate part $|\phi_0|^2$ combined G_ψ, gives a delta function contribution of magnitude $|\phi_0|^2$ dispersing with the free fermion dispersion. The phonon contribution leads to a continuous spectrum rising linearly with ω. Another continuous contribution onsets above the energy gap of the amplitude (or Higgs) mode. All three features are seen in Fig. 3(a), where the spectral function $A(k, \omega)$ at $k = k_F$ has been calculated for $c/v_F = 3$ and a quadratic fermionic dispersion $\epsilon_k = k^2/2$.

Upon approaching the critical point, the quasiparticle weight $Z \sim |\phi_0|^2 \sim U_{bb}^c - U_{bb}$ decreases to zero. Correspondingly, a pseudogap develops in the local density of states, see inset of Fig. 3(a). Directly at criticality, $U_{bb} = U_{bb}^c$, where $Z = 0$, the spectral function at $k = k_F$ rises linearly in ω, see Fig. 3(a). The underlying quadratic dispersion of the composite fermions and the linear dispersion of the bosonic excitations are clearly visible in Fig. 3(b).

Finally, inside the Mott phase the bosonic fluctuations can be treated as a free massive field. Hence, upon convolution with G_ψ one obtains a fully gapped spectral function despite the existence of a gapless Fermi liquid.

The gapless fermions of the Mott insulator are hidden from standard single particle probes such as photoemission or the momentum distribution measured in time of flight. Interestingly, however, the hidden Fermi surface can be revealed by noise correlations in time of flight images [19]. The boson-fermion cross correlations at momenta $\mathbf{k}$ and $\mathbf{k} + \mathbf{q}$ are directly proportional to the momentum-$\mathbf{q}$ distribution of the *composite fermions*,

$$\langle n_{\mathbf{q}}^c \rangle \approx \sum_{\mathbf{k}} \langle n_{\mathbf{k}+\mathbf{q}}^f n_{\mathbf{k}}^b \rangle - \langle n_{\mathbf{k}+\mathbf{q}}^f \rangle \langle n_{\mathbf{k}}^b \rangle. \qquad (8)$$

The approximation becomes exact deep in the Mott insulating state, where $f_i^\dagger b_j = \delta_{ij} c_i^\dagger$ for U_{bf}, $U_{bb} \to \infty$. The composite Fermi surface can also be observed by Bragg or lattice modulation probes that couple asymmetrically to bosons and fermions. The appropriate structure factors will display a gapless spectrum in the composite Fermi liquid phase or a small gap in case of p-wave pairing.

Conclusions.—Mixed boson-fermion systems in optical lattices open a new route, for both theoretical and experimental investigation of unconventional Mott transitions that entail the destruction of fermionic quasiparticles and the emergence of hidden Fermi surfaces of composite particles. We presented a theory that accounts for the critical behavior of the single fermion spectral function and gives a simple and tractable example for the emergence of a pseudogap in a strongly correlated system. While for $d = 3$, the nature of the phase transition depends on the ratio of the interactions, see Fig. 1, it has been shown that in $d = 1$ always a single $z = 1$ transition is expected [20].

An interesting open question is the nature of the possible tricritical point postulated in Fig. 1 where $U_{bb} \approx U_{bf}$ and two $z = 2$ transitions meet with the $z = 1$ critical point. Interestingly, the generalized Hubbard model (1) exhibits supersymmetry at $U_{bb} = U_{bf}$, $\mu_b = \mu_f$ and $t_f = t_b$ [21]. The ground state at the super-symmetric point has no fermions but may help to elucidate the nature of the tricritical point for low fermion density. Another open question concerns the Mott transition in a commensurate mixture of bosons and spinfull fermions.

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