Stability and Pairing in Quasi-One-Dimensional Bose-Fermi Mixtures

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We consider a mixture of single-component bosonic and fermionic atoms in an array of coupled one-dimensional "tubes." For an attractive Bose-Fermi interaction, we show that the system exhibits phase separation instead of the usual collapse. Moreover, above a critical intertube hopping, all first-order instabilities disappear in both attractive and repulsive mixtures. The possibility of suppressing instabilities in this system suggests a route towards the realization of paired phases, including a superfluid of p-wave pairs unique to the coupled-tube system, and quantum critical phenomena.

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Recently, heteronuclear resonances in mixtures of bosonic and fermionic ultracold atoms have attracted noticeable theoretical and experimental interest, due to the possibility of generating and exploring novel quantum phenomena in a controllable manner. For example, by varying the interaction in a Bose-Fermi (BF) mixture, one can, in principle, observe a quantum phase transition from a Bose-Einstein condensate (BEC) to a normal Fermi gas phase by binding bosons and fermions into fermionic molecules [1,2]. Indeed, this feature has already been exploited to create deeply bound, polar fermionic molecules [3]. However, the single biggest impediment to realizing such novel phenomena in BF mixtures is substantial inelastic collisions. The situation is particularly severe on the attractive side of the heteronuclear resonance, where a collapse of the cloud has been observed [4,5], resulting in a sudden loss of atoms from three-body recombination. On the repulsive side of the resonance, an interaction-induced spatial separation of bosons and fermions [6,7] ensures that the atomic system is relatively stable [8,9]. However, if one sweeps through the resonance, the system once again suffers significant inelastic losses when molecules collide with atoms [10].

In this Letter, we argue that many of these obstacles may be circumvented by embedding the mixture in a two-dimensional (2D) array of 1D tubes generated via an anisotropic optical lattice. Such a lattice is experimentally realizable and has already been used to explore the 1D-3D crossover in a Bose gas [11]. While strictly 1D BF mixtures have been investigated extensively in several theoretical works [12–20], the novelty of our approach is to allow a finite hopping between tubes, thus preserving the true long-range order of condensed phases as found in 3D, while still maintaining the advantages of a 1D system. In particular, 3-body recombination should be greatly reduced, perhaps even more than in a BF mixture confined to a 3D optical lattice (see, e.g., [21]), since its rate *vanishes* for short-ranged interactions in the 1D limit [22]. Furthermore, we demonstrate using mean-field theory that, similarly to 1D [16] and contrary to expectation [14,20], there is no collapse in a quasi-1D attractive mixture. Crucially, we find that the hopping can be used to suppress first-order instabilities in BF mixtures and, as such, it may allow one to investigate quantum phase transitions induced by BF pairing [1,2], without the intrusion of first-order transitions. In addition, we will show using the Luttinger liquid formalism that, for a sufficiently strong BF attraction, the coupled-tube system exhibits an exotic superfluid phase, where p-wave pairing occurs between fermionic molecules composed of a single boson and a single fermion.

In the following, we consider a mixture of bosonic (b) and fermionic (f) atoms confined in an $N_x \times N_y$ square array of 1D tubes of length L_z. We focus on the homogeneous case, but our results can easily be mapped to the case of a harmonic trapping potential using the local density approximation [6]. For sufficiently strong lattice confinement, the xy motion can be approximated by a single-band, tight-binding model (setting $\hbar = 1$),

$$\epsilon_{\mathbf{k}}^{f,b} = \frac{k_z^2}{2m_{f,b}} + 2t[2 - \cos(k_x d) - \cos(k_y d)], \quad (1)$$

where t is the hopping between tubes and d is the tube spacing. Here, the transverse xy momenta are restricted to the first Brillouin zone, $|k_{x,y}| \leq \pi/d$. The single-channel Hamiltonian is thus

$$\hat{H} = \sum_{\mathbf{k}} (\xi_{\mathbf{k}}^f f_{\mathbf{k}}^\dagger f_{\mathbf{k}} + \xi_{\mathbf{k}}^b b_{\mathbf{k}}^\dagger b_{\mathbf{k}}) + \frac{1}{L_z N_x N_y} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \Big[U_{\mathrm{BF}} b_{\mathbf{k}}^\dagger f_{\mathbf{k}'}^\dagger f_{\mathbf{k}'+\mathbf{q}} b_{\mathbf{k}-\mathbf{q}} + \frac{U_{\mathrm{BB}}}{2} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'}^\dagger b_{\mathbf{k}'+\mathbf{q}} b_{\mathbf{k}-\mathbf{q}} \Big], \quad (2)$$

where $\xi_{\mathbf{k}}^{f,b} = \epsilon_{\mathbf{k}}^{f,b} - \mu_{f,b}$ and μ_f (μ_b) is the fermionic (bosonic) chemical potential. The contact interactions U_{BF}, U_{BB} are effectively 1D, and we choose a repulsive boson-boson interaction $U_{\mathrm{BB}} > 0$ to ensure the stability of the Bose gas. Interactions between identical fermions can be neglected due to the Pauli exclusion principle. If all atoms experience the same transverse trapping frequency $\omega_\perp$, then the 1D interactions $U_{\rm BF}$ and $U_{\rm BB}$ can be written simply in terms of the 3D scattering lengths $a_{\rm BF}$ and $a_{\rm BB}$ [23]:

$$\frac{1}{U_{\alpha\beta}} = \frac{m_{\alpha\beta}a_{\alpha\beta\perp}}{2}\left(\frac{a_{\alpha\beta\perp}}{a_{\alpha\beta}} - C\right), \quad (3)$$

where the oscillator length of the tube $a_{\alpha\beta\perp} = \sqrt{1/m_{\alpha\beta}\omega_\perp}$ depends on the masses $m_{\rm BB} \equiv m_b$ and $m_{\rm BF} = 2m_f m_b/(m_f + m_b)$, while $C \simeq 1.4603/\sqrt{2}$.

The introduction of an intertube hopping t naturally leads to a crossover from 1D to 3D behavior. The limit $\epsilon_{\mathbf{k}}^{f,b} \ll t$ recovers the isotropic 3D dispersion, while the opposite limit $\epsilon_{\mathbf{k}}^{f,b} \gg 8t$ corresponds to the 1D regime. For degenerate fermions, this implies 3D behavior when the Fermi energy $\varepsilon_F \ll t$, i.e., at sufficiently small densities, and 1D behavior when $\varepsilon_F \gg 8t$, i.e., at large densities. However, for weakly interacting degenerate bosons, the spread of the momentum distribution is set by the temperature T and thus we require $k_BT \ll t$ and $k_BT \gg 8t$, respectively, to access the 3D and 1D regimes. A corollary of this is that we expect the superfluid critical temperature T_c of the quasi-1D Bose gas to be finite and scale as some positive power of t. Contrast this with the strictly 1D limit ($t = 0$), where T_c is strictly zero. We shall focus on the $T = 0$ limit, so the effective dimensionality will only depend on the fermion density.

We begin by analyzing the first-order instabilities of the quasi-1D mixture using mean-field theory. Of course, for purely 1D mixtures, a mean-field description [13,16] is unreliable because the physics is dominated by fluctuations, and one must instead use the Luttinger liquid formalism [14]. However, we expect a mean-field treatment to be reasonable for finite intertube hopping, because then it works well in the low-density 3D limit ($t/\varepsilon_F \gg 1$), as well as being consistent with the Luttinger liquid description in the high-density, weak-coupling, 1D regime ($8t/\varepsilon_F \ll 1$, $|U_{\rm BF}|\sqrt{2m_f/\varepsilon_F} \ll 1$) [14]. Specifically, we take $b_{\mathbf{k}} = \delta_{\mathbf{k},0}\sqrt{L_zN_xN_y}\Phi$, so that the grand-canonical free energy density $\Omega(\mu_f, \mu_b) = \min_\Phi f(\Phi, \mu_f, \mu_b)$ can be easily evaluated by integrating out the fermionic degrees of freedom, giving

$$f = -\frac{1}{N_xN_y}\sum_{k_x,k_y}^{B.z.}\frac{2}{3\pi}\frac{k_{Fz}^3}{2m_f} - \mu_b\Phi^2 + \frac{U_{\rm BB}}{2}\Phi^4,$$
$$\frac{k_{Fz}^2}{2m_f} = \mu_f - U_{\rm BF}\Phi^2 - 2t[2 - \cos(k_xd) - \cos(k_yd)]. \quad (4)$$

In addition, the 1D densities of fermions and bosons in each tube are given, respectively, by $n_b = \Phi^2$ and $n_f = 1/(N_xN_y)\sum_{k_x,k_y}^{B.z.} k_{Fz}/\pi$, so that, within mean field, we always have a BEC when $n_b > 0$. Here, the system dimensionality is set by the parameter $(\mu_f - U_{\rm BF}\Phi^2)/t$ or, equivalently, $\pi n_f/\alpha\sqrt{2tm_f}$, where $\alpha = \int_0^\pi dk_xdk_y\sqrt{2 + \cos k_x + \cos k_y}/\pi^2 \simeq 1.35$.

For a 3D, attractive ($U_{\rm BF} < 0$) mixture with no optical lattice, it is easy to see that the free energy at large Φ is dominated by the BF interaction term ($\propto -\Phi^5$ in 3D) and is thus not bounded from below [24]. This implies that the system is unstable to collapse at sufficiently high densities [7,25]. On the other hand, in a 1D tube, the interaction term instead scales like $-\Phi^3$ at large Φ and is thus compensated by the boson-boson repulsion ($\propto \Phi^4$) [16]. Therefore, contrary to what has been previously assumed [14,20], both 1D and quasi-1D attractive BF mixtures will exhibit phase separation instead of collapse.

After minimizing the free energy (4) with respect to the boson field Φ, we can construct the phase diagram using just three dimensionless parameters, such as the dimensionless hopping strength $t' \equiv 2m_ft/c_f^2$, and the dimensionless densities $n_{b,f}/c_{b,f}$, where $c_b = 2m_f|U_{\rm BF}|^3/(\pi^2U_{\rm BB}^2)$, $c_f = 2m_fU_{\rm BF}^2/(\pi^2U_{\rm BB})$. The repulsive, strictly 1D ($t = 0$) case has been evaluated within mean field in Ref. [13]: here, contrary to the 3D case [7], phase separation occurs at *low* fermionic densities, $n_f/c_f \le 3/4$, irrespective of the boson density. Furthermore, phase separation only occurs between two pure phases (when $n_b/c_b \le 3/4$) or between a mixed phase and a purely bosonic phase (when $n_b/c_b > 3/4$). The topology of the repulsive phase diagram changes substantially once $t > 0$. As shown in Fig. 1, a stable tricritical point [26] appears at low fermionic densities and there is instead a uniform phase for $n_f/\sqrt{2tm_f} \ll \alpha/\pi$. Here, the phase diagram resembles the 3D phase diagram derived in Ref. [7], as expected. By contrast, at higher fermionic densities, we recover 1D behavior, such that phase separation only exists for $n_f/c_f \lesssim$ const. However, we note that there is never phase separation between two pure phases at finite t, unlike in the strictly 1D and 3D cases. Instead, phase separation either occurs between a purely fermionic and a mixed phase (for $n_f/c_f < 0.73$ and $n_b/c_b < 0.73$ in Fig. 1) or between two mixed phases.

For the attractive case, the structure of the phase diagram does not change when hopping is switched on. Moreover, unlike the 3D case, the mixture displays phase separation instead of collapse, as previously discussed. However, the phase diagram has a region where phase separation occurs between a mixed phase and the vacuum (see Fig. 1), and this may be viewed as a remnant of the collapse in the 3D system. Note that the tricritical points have the same values as in a repulsive mixture at the same t', but their stability is switched. Both attractive and repulsive mixtures at the same t' also feature identical spinodal lines [27], which

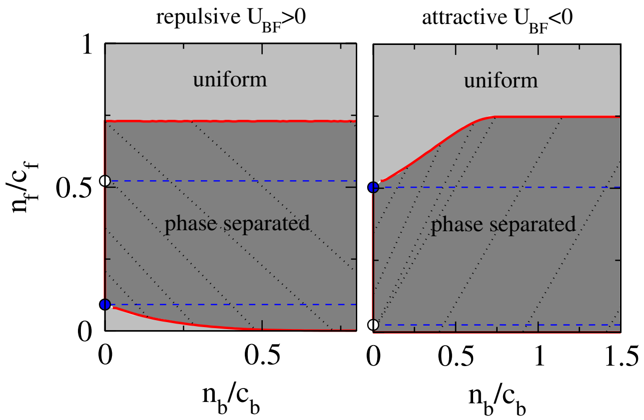

FIG. 1 (color online). Zero temperature, mean-field phase diagrams in density space for a repulsive BF mixture with dimensionless hopping strength $t' \equiv 2m_f t/c_f^2 = 0.5$ (left panel), and an attractive mixture with $t' = 0.2$ (right). Each mixture can either form a uniform BEC phase (light gray shaded region) or it can undergo a first-order transition (thick red lines) to a phase-separated state (dark gray). The dotted lines connect points on the first-order boundary with the same chemical potential. Filled circles mark stable tricritical points, where 1st and 2nd ($n_b = 0$) order transition lines merge, while the empty circles correspond to unstable ones. Spinodal lines (blue dashed) divide the phase-separated region into the unstable domain (internal region) and the metastable domain (external). Note that, for the repulsive mixture, the phase at very low fermionic densities is always uniform.

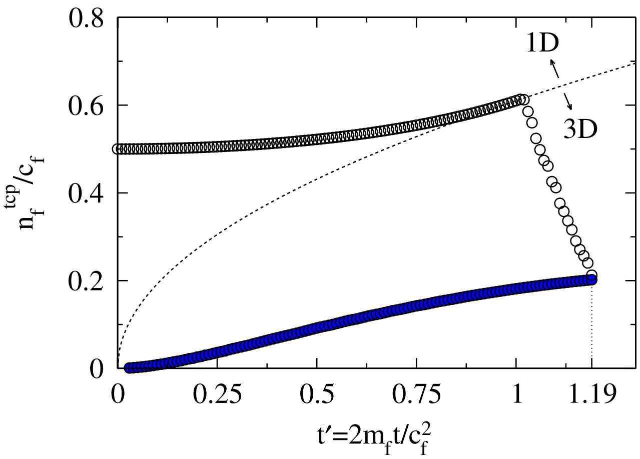

FIG. 2 (color online). Evolution of the stable (filled blue circles) and unstable (empty circles) tricritical points $n_f^{\rm tcp}/c_f$ ($n_b^{\rm tcp} = 0$) as a function of the hopping strength t' for a repulsive mixture. For attractive mixtures, the tricritical points have the same values, but the stable and unstable branches are switched. The (dashed) line approximately separating the 1D from the 3D regime is $n_f/c_f = \sqrt{2t'}\alpha/\pi$, with $\alpha \simeq 1.35$—this defines the point, $\mu_f - U_{\rm BF}\Phi^2 = 8t$, where the Fermi surface first touches the xy band edge. Tricritical points disappear altogether above the critical value $t'_{\rm cr} \simeq 1.19$.

indicate when the system becomes linearly unstable to phase separation.

By tracking the evolution of the stable and unstable tricritical points as a function of t' (Fig. 2), we find that the situation dramatically changes at larger t'. Notably, at the critical value $t'_{\rm cr} \simeq 1.19$, the stable and unstable tricritical points merge, and the width of the phase-separated region reduces to zero. Thus, for $t' > t'_{\rm cr}$, the system exhibits only a uniform phase. This is a consequence of the 1D-3D crossover in this system: eventually the instabilities of the 1D regime fall in the low density regime where 3D behavior dominates, and vice versa. These results suggest that one can stabilize a BF mixture using an appropriate 2D optical lattice. Indeed, we find that if the oscillator length $a_{\rm BB\perp}$ is comparable to the boson-boson scattering $a_{\rm BB}$, then we can have the situation where there is phase separation or collapse in 3D and yet no instabilities in the quasi-1D case for $t > t'_{\rm cr}$. This is basically because the effective 1D interaction $U_{\rm BB}$ diverges at $a_{\rm BB\perp} = Ca_{\rm BB}$ in Eq. (3).

The absence of collapse makes quasi-1D systems ideal for examining BF pairing. In particular, the possibility of suppressing first-order instabilities by tuning the hopping strength opens up the prospect of investigating quantum phase transitions. For example, one could realize a continuous quantum phase transition, where the BEC is destroyed by the pairing. Even though our mean-field treatment does not include the possibility of pairing, we can still get an estimate of the instability towards BF pairing by considering the two-body problem. In the $t = 0$ limit, the BF binding energy is approximately $\varepsilon = m_{\rm BF}U_{\rm BF}^2/4$, which becomes exact in the limit $|a_{\rm BF}| \to 0$ [28]. However, once we switch on the hopping, the bound state is lost when $t \simeq 0.05 m_{\rm BF}U_{\rm BF}^2$. Thus, if we wish to explore pairing-induced phase transitions in the absence of first-order instabilities, we need this "resonance" to lie above $t'_{\rm cr}$; i.e., we require $U_{\rm BB}/U_{\rm BF} \gtrsim 0.2(1 + m_f/m_b)$.

We can determine what symmetry-broken states may exist in the quasi-1D system by comparing the decay of different correlation functions in the purely 1D limit. On general grounds we expect that the operator with the slowest decay in 1D will fix the long-range ordering of the higher-dimensional system. This is due to the fact that the exponent η governing the spatial decay of the operator $\hat{\mathcal{O}}$, $\langle \hat{\mathcal{O}}_x \hat{\mathcal{O}}_0 \rangle \sim 1/x^\eta$, also appears in the susceptibility as a function of temperature, $\chi(T) \sim T^{\eta-2}$, and one can show using a mean-field approximation for the intertube couplings that the symmetry-broken state with the most divergent $\chi(T)$ generally has the highest T_c [29].

In the strictly 1D limit, the low-energy low-wavelength effective field theory is described by the Luttinger formalism (bosonization) [14]. In particular, we consider the case where the fermionic and bosonic phase velocities are similar $v_f = v_b = v$ and the low-energy effective Hamiltonian can be described by introducing in- and out-of-phase phase and density fluctuations of the mixture [14], $\phi_{1,2} = \frac{1}{\sqrt{2}} \times (\phi_b \pm \phi_f)$ and $\theta_{1,2} = \frac{1}{\sqrt{2}}(\theta_b \pm \theta_f)$:

$$H_{\rm eff} = \sum_{a=1,2} \frac{v_a}{2\pi} \int dx \Big[K_a (\partial_x \theta_a)^2 + \frac{1}{K_a} (\partial_x \phi_a)^2 \Big] + \frac{2U_{\rm BF}}{(2\pi\Lambda)^2} \int dx \cos 2[\sqrt{2}\phi_2 - \pi(n_f - n_b)x], \quad (5)$$

where $K_{1,2}$ are Luttinger parameters and Λ a cutoff. The in-phase mode 1 describes a one-component (gapless) Luttinger liquid. We emphasize that Eq. (5) holds for any value of the BF coupling. However, $K_{1,2}$ can only be determined analytically in the limit of small $U_{\rm BF}$ and one must resort to numerics [20] when a perturbative expansion in $U_{\rm BF}$ is no longer accurate.

In the limit of equal filling, $n_f = n_b$, the field ϕ_2 acquires a gap—the corresponding "paired" phase has been introduced in Ref. [14]. The slowest algebraic decay is then given by the operator $\hat{\mathcal{O}} = bf$ when $K_1 > 2/\sqrt{3}$; otherwise it is given by charge-density wave correlations. However $\hat{\mathcal{O}}$ is a *fermionic* operator and as such cannot lead to condensation when we couple the tubes to access the 3D limit. Instead we must consider the composite *bosonic* operator $\hat{\mathcal{O}}^{(n)} = f_L f_R b^n$, whose correlations can be evaluated from Eq. (5):

$$\hat{\mathcal{O}}^{(n)} \propto e^{i[\sqrt{2}+(n/\sqrt{2})]\theta_1 + i[-\sqrt{2}+(n/\sqrt{2})]\theta_2}. \quad (6)$$

In the paired phase the field ϕ_2 is pinned by the relevance of the cosine operator in Eq. (5) and therefore the conjugate field θ_2 has exponentially decaying correlations. As a consequence, $\hat{\mathcal{O}}^{(n)}$ also has exponentially decaying correlations unless $n = 2$. Equation (6) leads to a decay law $\langle \hat{\mathcal{O}}_x^{(2)} \hat{\mathcal{O}}_0^{(2)} \rangle \sim 1/x^{4/K_1}$ and dominates over charge-density wave correlations for $K_1 > 2$. Therefore, in a system of weakly coupled tubes we expect condensation of the operator $\hat{\mathcal{O}}^{(2)}$, i.e., a p-wave paired phase of fermionic molecules each composed of a single boson and a single fermion. In the strictly 1D system, this operator was recognized to have quasi-long-range order in Ref. [19]. Here, we find that, for $K_1 > 2$, the operator $\hat{\mathcal{O}}^{(2)}$ has the slowest decaying correlations and therefore implies condensation of fermionic molecules in the higher-dimensional system. Moreover, the p-wave phase of fermionic molecules is topologically distinct from a superfluid of p-wave pairs of atomic fermions coexisting with a BEC. In the former, even though the global phase symmetry is broken, there is a remaining subgroup $U(1)_{B-F}$ of relative phase transformations between bosons and fermions that is preserved, since b^2 and $f_L f_R$ can be rotated by opposite phase factors without changing the superfluid order parameter. The p-wave order parameter $\Delta_{\mathbf{k}}$ also breaks full spatial rotation symmetry $SO(3)$ and, in the ground state, can either be of the form $\Delta_{\mathbf{k}} \propto k_z$ (a spinless equivalent of the polar phase of superfluid ^{3}He) or $\Delta_{\mathbf{k}} \propto k_x + ik_y$ (the spinless variant of the ^{3}He A phase). Finally, we note that it should be possible to access this p-wave phase in an attractive BF mixture: a numerical DMRG analysis for ^{40}K-^{87}Rb mixtures [20] has shown that deep inside the paired phase there is at least one point with $K_1 \sim 2$.

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