Fermi-Bose Mixtures near Broad Interspecies Feshbach Resonances

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In this Letter we study dressed bound states in Fermi-Bose mixtures near broad interspecies resonances, and implications on many-body correlations. We present the evidence for a first order phase transition between a mixture of Fermi gas and condensate, and a fully paired mixture where extended fermionic molecules occupy a single pairing channel instead of forming a molecular Fermi surface. We further investigate the effect of Fermi surface dynamics and pair fluctuations and discuss the validity of our results.

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Since the observation of molecules of Fermi atoms near Feshbach resonances, fascinating pairing correlations in cold Fermi gases have been successfully investigated both experimentally [1–5] and theoretically [6–8]. Near broad resonances where the atom-molecule coupling is very strong, pair correlations can also be closely related to the ones in the crossover theory pioneered a while ago [9–11]. Meanwhile, interspecies Feshbach resonances in Fermi-Bose mixtures of ^{6}Li-^{23}Na, ^{40}K-^{87}Rb, and ^{6}Li-^{87}Rb have been experimentally observed [12–16]. Recently, weakly bound ^{40}K-^{87}Rb pairs prepared near Feshbach resonances were further successfully converted into cold molecules [17], which can potentially lead to exciting opportunities for studying new quantum states of matter [18]. Previous theoretical studies on Fermi-Bose mixtures, on the other hand, have mainly focused on narrow resonances or when the atom-molecule coupling is very weak [19–21]; phase boundaries in this limit depend on atom-molecule coupling strengths.

Experimentally, creating and probing correlations in Fermi-Bose mixtures near narrow resonances is more challenging than near broad resonances. For a Feshbach resonance with a width ΔB and background scattering length a_{BG}, an effective resonance energy width can be introduced as $\Gamma_{\mathrm{res}} = 2m_R a_{\mathrm{BG}}^2(\Delta\mu\Delta B)^2/\hbar^2$; here $\Delta\mu$ is the difference in magnetic moments between the scattering and molecule channels and m_R is the reduced mass of a pair of Bose and Fermi atoms. For interspecies resonances confirmed so far [12–16,23], Γ_{res} can be a few orders of magnitude bigger than the Fermi energy at a typical density of 10^{14} cm^{-3} [12]. So some of the well-studied resonances are quite broad, and many-body correlations near these interspecies resonances are still not thoroughly understood. One of the very fundamental questions we hope to answer in this Letter is, what is the nature of quantum matter near broad interspecies resonances. In particular, how do dressed two-body bound states evolve when approaching resonances? Accordingly, what kinds of many-body correlations are developed in a quantum Fermi-Bose mixture? And the physics near broad resonances can distinctly differ from that near narrow resonances; some basic concepts introduced for narrow resonances such as molecular Fermi surfaces might not be directly applicable here. Motivated by these considerations, we carry out a study on Fermi-Bose mixtures near broad interspecies Feshbach resonances, which serves as a potential reference for more sophisticated analyses. Apart from the phase diagrams in terms of interspecies scattering lengths a_{bf} and the Bose-Fermi mass ratio m_B/m_F, we focus on bound state properties which can be potentially probed in experiments. Our results are useful for the understanding of correlations in ^{6}Li-^{23}Na, ^{6}Li-^{87}Rb, and ^{40}K-^{87}Rb mixtures. For simplicity, we employ a simplest one-channel Hamiltonian which captures the most important aspects near broad resonances,

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^F f_{\mathbf{k}}^\dagger f_{\mathbf{k}} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^B b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \frac{V_{\mathrm{bf}}}{\Omega} \sum_{\mathbf{k},\mathbf{k}',\mathbf{Q}} f^\dagger_{(m_R/m_B)\mathbf{Q}+\mathbf{k}} \times b^\dagger_{(m_R/m_F)\mathbf{Q}-\mathbf{k}} f_{(m_R/m_B)\mathbf{Q}+\mathbf{k}'} b_{(m_R/m_F)\mathbf{Q}-\mathbf{k}'}, \tag{1}$$

where $f_{\mathbf{k}}^\dagger$, $b_{\mathbf{k}}^\dagger$ ($f_{\mathbf{k}}$, $b_{\mathbf{k}}$) are creation (annihilation) operators for Fermi and Bose atoms, respectively; $\epsilon_{\mathbf{k}}^{F(B)} = \frac{\hbar^2|\mathbf{k}|^2}{2m_{F(B)}}$ are kinetic energies for fermions (bosons) and Ω is the volume. V_{bf} is the strength of the interaction that is related to interspecies scattering lengths a_{bf} via

$$\frac{1}{V_{\mathrm{bf}}} = \frac{m_R}{2\pi a_{\mathrm{bf}}\hbar^2} - \frac{1}{\Omega}\sum_{\mathbf{k}} \frac{1}{\epsilon_{\mathbf{k}}^R}; \tag{2}$$

here $m_R = m_B m_F/(m_B + m_F)$, $\epsilon_{\mathbf{k}}^R = \hbar^2\mathbf{k}^2/2m_R$. We assume that the background boson-boson interactions are repulsive so that the mixture is stable; to illustrate the idea, here we only include interspecies scattering.

We first consider the binding energy of a pair of Fermi and Bose atoms with opposite momenta ($\mathbf{k}$, $-\mathbf{k}$) in the presence of a condensate (BEC) and a Fermi surface of Fermi atoms which blocks all states below its Fermi momentum $\hbar k_F$. Pauli blocking effects of a Fermi sea indeed lead to *dressed* bound states at arbitrarily small negative scattering lengths but with an anomalous dispersion or a negative effective mass [see also the discussions before

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Eq. (4)]. Furthermore, the energy W_B it takes to create a bound state from a noninteracting ground state can be either positive or negative depending on the scattering lengths $a_{\rm bf}$, a unique feature of Fermi-Bose systems. This is because, to form a pair of atoms with opposite momenta $(\mathbf{k}, -\mathbf{k})$ near the Fermi surface $|\mathbf{k}| = k_F$, a Bose atom has to be promoted to right above the Fermi surface, which results in an energy penalty of $\epsilon_F^B = \hbar^2 k_F^2/2m_B$. For a bound state with an arbitrary total momentum $\mathbf{Q}$ or a kinetic energy $\epsilon_{\mathbf{Q}}^C = \hbar^2\mathbf{Q}^2/2(m_F + m_B)$, the energy cost is $W_B(\mathbf{Q}) = \epsilon_F^B + \epsilon_{\mathbf{Q}}^C + \omega_B$. The $\mathbf{Q}$-dependent $\omega_B(<0)$ can be obtained by solving the equation

$$\frac{-m_R\Omega}{2\pi a_{\rm bf}\hbar^2} = \left(\sum_{|(m_R/m_B)\mathbf{Q}+\mathbf{k}|>k_F} \frac{1}{\epsilon_{\mathbf{k}}^R - \epsilon_F^R - \omega_B} - \sum_{\mathbf{k}} \frac{1}{\epsilon_{\mathbf{k}}^R}\right). \tag{3}$$

In the limit of small $k_F a_{\rm bf}(<0)$ and when $\mathbf{Q} = 0$, Eq. (3) leads to $\omega_B = -4\epsilon_F^R \exp(\frac{\pi}{k_F a_{\rm bf}})$, $\epsilon_F^R = \hbar^2 k_F^2/2m_R$. The dispersion of bound states that can be probed using photoassociative spectroscopy is shown in Fig. 1. For small negative scattering lengths $a_{\rm bf}$, bound states are fully gapped with positive energies $W_B(\mathbf{Q})$, and the ground state is a mixture of Fermi gas and BEC. However, $W_B(0)$, the energy gap of bound states, vanishes at a *critical* scattering length $a^{(1)}$. In Fig. 2, we present results of $a^{(1)}$ versus m_B/m_F. For heavy Bose atoms, $k_F a^{(1)}$ approaches a small value of $\pi/\ln[m_F/4m_B]$.

To ensure the stability of $\mathbf{Q} = 0$ molecules near the transition line $a^{(1)}$, we further examine $M_{\rm eff}$, the effective mass near $\mathbf{Q} = 0$. At scattering lengths $a^{(1)}$ or when $W_B(0) = 0$, we find

$$\frac{1}{M_{\rm eff}} = \frac{1}{m_T}\left[1 - \frac{4m_F}{3m_B} g\left(\frac{m_R}{m_F}\right)\right], \tag{4}$$

and the dimensionless function $g(x^2) = x/[(1-x^2)^2 \times (\ln\frac{1+x}{1-x} + \frac{2x}{1-x^2})]$. As long as $m_B/m_F > 0.7$ and the energy penalty ϵ_F^B is not too heavy, $M_{\rm eff}$ is positive, although it can be much bigger than the bare mass $m_T(= m_F + m_B)$ as a result of dressing in the Fermi sea. Below we focus on the limit of positive $M_{\rm eff}$ that is most relevant to the experimental mass ratio m_B/m_F (between 2.175 and 14.5) [24]. Note that the binding energy ω_B is independent of the Bose atom density when the Fermi sea is treated as a static background.

The above analysis, at first sight, seems to suggest that when W_B becomes negative, a small fraction of Fermi and Bose atoms start forming molecules or a dilute molecular Fermi gas signifying a phase transition at $a^{(1)}$. Such a picture was in fact previously proposed for mixtures near *narrow* resonances [19,20]. However, since the extent of molecules d_m is typically comparable to or much longer than the Fermi wavelength $2\pi/k_F$ near broad resonances, pairs may be accommodated, even before the two-body gap W_B vanishes, in other more exotic forms without forming a molecular Fermi surface. Below we provide evidence for such a possibility. Note that a finite two-body gap W_B suggests a local stability of the Fermi gas-BEC mixture against the emergence of a Fermi gas of molecules; i.e., when $1/a < 1/a^{(1)}$, a molecular Fermi gas *cannot* be a ground state. It is in this limit that we illustrate, based on an energetic analysis, that a *third* state or a fully paired state actually further lowers the energy.

Suggested by the above discussions, we consider the energetics of pairing states of Fermi-Bose atoms and, from now on, focus on *homogeneous* mixtures with equal populations of fermions and bosons, i.e. $N_F = N_B$. Although, in principle, pairing with a finite total momentum $\hbar\mathbf{Q}$ can occur in ground states, detailed calculations show that, for a range of mass ratios $(m_B/m_F > 0.2)$ relevant to Fermi-Bose mixtures studied in experiments

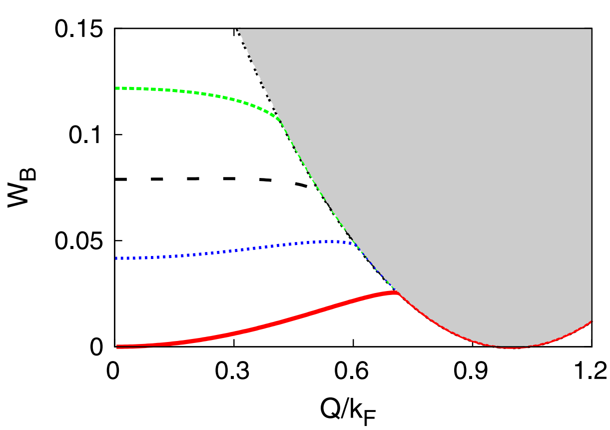

FIG. 1 (color online). The energy dispersion of bound states for the mass ratio $m_B/m_F = 2.175$ or ^{40}K-^{87}Rb mixtures. From top to bottom the lines represent $W_B(\mathbf{Q})$ in units of ϵ_F^R for $1/k_F a_{\rm bf} = -0.2$, -0.1145, -0.05, and 0.0145. The shaded region represents the pair excitation continuum.

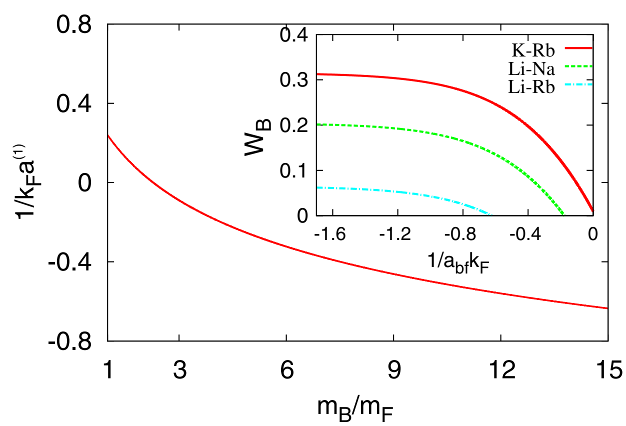

FIG. 2 (color online). Scattering length $a^{(1)}$ at which the energy cost W_B to create a molecule with $\hbar\mathbf{Q} = 0$ from a Fermi gas-BEC mixture becomes zero, as a function of the Bose-Fermi mass ratio m_B/m_F. The inset shows W_B, the energy gap of molecules in units of ϵ_F^R as a function of $k_F a_{\rm bf}$ (and $1/a_{\rm bf} < 1/a^{(1)}$) for different mass ratios or mixtures.

so far, pairing in the $\hbar\mathbf{Q}=0$ channel is always dominant and favored, qualitatively consistent with our analyses on the two-body bound states. Below we only show results of $\mathbf{Q}=0$ pairing and adopt the simplest pairing wave function

$$|\mathrm{g.s.}\rangle = \exp(c_0 b_0^\dagger)\prod_k (u_{\mathbf{k}} + v_{\mathbf{k}} f_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + \eta_{\mathbf{k}} f_{\mathbf{k}}^\dagger)|\mathrm{vac}\rangle, \quad (5)$$

where $u_{\mathbf{k}}$, $v_{\mathbf{k}}$, and $\eta_{\mathbf{k}}$ are three families of variational parameters. We obtain the energy of the variational states and then minimize it with respect to $u_{\mathbf{k}}$, $v_{\mathbf{k}}$, and $\eta_{\mathbf{k}}$, which are subject to the normalization condition $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 + |\eta_{\mathbf{k}}|^2 = 1$. Equilibrium conditions can then be obtained, and there are two solutions for any given $\mathbf{k}$: (i) an unpaired state with $\eta_{\mathbf{k}} = 1$ and $u_{\mathbf{k}} = v_{\mathbf{k}} = 0$ and (ii) a paired state with $\eta_{\mathbf{k}} = 0$ and $v_{\mathbf{k}}^2 = \frac{1}{2}(1 - \frac{\xi_{\mathbf{k}}^R}{E_{\mathbf{k}}})$, $u_{\mathbf{k}}^2 = \frac{1}{2}(1 + \frac{\xi_{\mathbf{k}}^R}{E_{\mathbf{k}}})$, and $\Delta = -\frac{V_{\mathrm{bf}}}{\Omega}\sum_{\mathbf{k}}(1-\eta_{\mathbf{k}}^2)u_{\mathbf{k}}v_{\mathbf{k}}$, where $E_{\mathbf{k}} = \sqrt{(\xi_{\mathbf{k}}^R)^2 + 4\Delta^2}$, $\xi_{\mathbf{k}}^R = \epsilon_{\mathbf{k}}^R - \mu$, and μ is the pair chemical potential. The pairing gap Δ, μ and the condensed population $|c_0|^2$ are determined self-consistently, $N_F = \sum_{\mathbf{k}}(v_{\mathbf{k}}^2(1-\eta_{\mathbf{k}}^2) + \eta_{\mathbf{k}}^2)$, $N_B = |c_0|^2 + \sum_{\mathbf{k}} v_{\mathbf{k}}^2(1-\eta_{\mathbf{k}}^2)$, and

$$\frac{-m_R\Omega}{2\pi a_{\mathrm{bf}}\hbar^2} = \sum_{\mathbf{k}} \frac{1-\eta_{\mathbf{k}}^2}{\sqrt{(\epsilon_{\mathbf{k}}^R - \mu)^2 + 4\Delta^2}} - \sum_{\mathbf{k}} \frac{1}{\epsilon_{\mathbf{k}}^R}. \quad (6)$$

To minimize the energy, we further choose $\eta_{\mathbf{k}}$ to be a step function, $\eta_{\mathbf{k}} = 1$ if $|\mathbf{k}| \leq Xk_F$, and zero otherwise; the dimensionless variational parameter $X \in [0, 1]$ specifies the size of the residue Fermi surface of unpaired Fermi atoms. When $N_F = N_B$, one can also verify that X^3 is equal to $|c_0|^2/N_B$, i.e., the condensation fraction.

In Figs. 3 and 4, we present the main results of variational calculations. In Fig. 3, the energy per pair of atoms is shown as a function of X, the size of the Fermi surface of unpaired fermions. At small and negative scattering lengths, a Fermi gas-BEC mixture is a ground state, and $X_0 = 1$, $\mu = \epsilon_F^F + W_B$ ($\epsilon_F^F = \hbar^2 k_F^2/2m_F$), and $\Delta = 0$. A fully paired state with $X_0 = 0$ becomes degenerate with the Fermi gas-BEC mixture ($X_0 = 1$) at a critical scattering length a_{cr}, beyond which the paired state becomes a ground state. However, a Fermi gas-BEC mixture remains locally stable until scattering lengths reach the value of $a^{(1)}$ which is fully consistent with the above study of bound states. Our variational calculations suggest a first order phase transition between a Fermi gas-BEC mixture and a fully paired mixture. This later state of extended molecules is conceptually different from a Fermi gas of molecules; instead, all molecules, though fermionic in nature, occupy the same pairing channel with zero total momentum. A direct comparison of energies indicates that a fully paired mixture has lower energies than a Fermi gas of molecules, provided $1/a_{\mathrm{bf}} < 1/a^{(2)}$. For ^{40}K-^{87}Rb mixtures, $1/k_F a^{(2)}$ is about 0.25–0.3 and $1/a^{(2)} > 1/a^{(1)}$; further towards the molecular side, a paired mixture is expected to evolve into a Fermi gas of molecules.

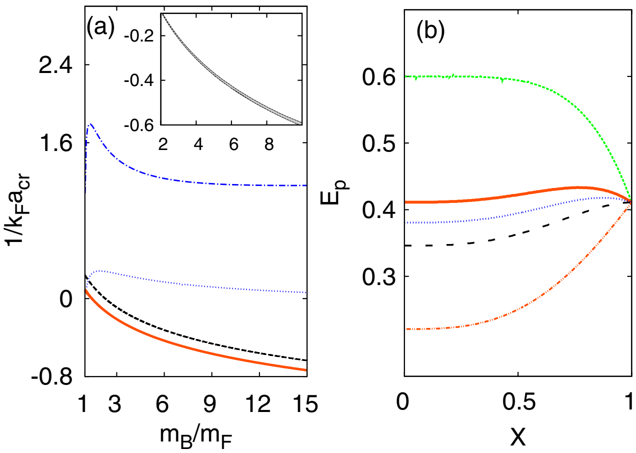

FIG. 3 (color online). (a) a_{cr} at which a first order phase transition occurs, as a function of the mass ratio m_B/m_F. The dashed line is $a^{(1)}$ along which a Fermi gas-BEC mixture becomes locally unstable. Near a_{cr}, there is a tiny window for phase separation (shaded area in the inset). The dotted (dashed-dotted) line is the shifted a_{cr} ($a^{(1)}$) due to quantum fluctuations [see the discussions around Eq. (7)]. (b) E_p, energy per pair of Fermi-Bose atoms in units of ϵ_F^R as a function of X, the size of the Fermi surface of unpaired Fermi atoms, for the $m_B/m_F = 2.175$ or ^{40}K-^{87}Rb mixture. From top to bottom, the lines represent E_p for $1/k_F a_{\mathrm{bf}} = -5$, -0.1145 (for a_{cr}), -0.05, 0.0145 (for $a^{(1)}$), and 0.2. $X = 1$ corresponds to an unpaired state, and $X = 0$ is for a fully paired mixture.

In Fig. 4, we further present the results on the pair-breaking energy Δ and the pair chemical potential μ. The pair-breaking energy can be probed when applying rf pulses to transfer Fermi atoms to a different hyperfine spin state [5,25] that weakly interacts with the Fermi-Bose mixture. The frequency shift in the rf spectroscopy should be $\hbar\Delta\omega(\mathbf{k}) = \frac{1}{2}(\xi_{\mathbf{k}}^R + \sqrt{|\xi_{\mathbf{k}}^R|^2 + 4\Delta^2})$. In the fully paired phase, Bose atoms are completely depleted and the Bose atom distribution $n_B(\mathbf{k})$ closely follows the Fermi atom distribution $n_F(\mathbf{k})$.

At small negative scattering lengths when quantum fluctuations are weak, our mean-field analyses on two-body bound states as well as the fully paired states are

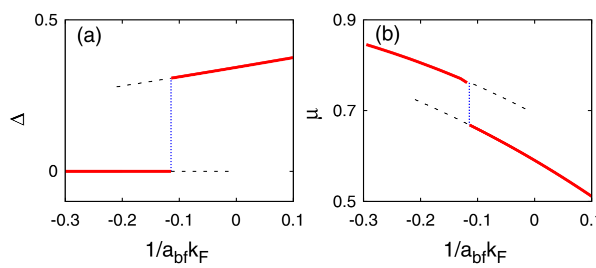

FIG. 4 (color online). (a) Pair-breaking energy Δ and (b) pair chemical potential μ in units of ϵ_F^R as a function of the scattering length $k_F a_{\mathrm{bf}}$ (near a_{cr}) for the mass ratio $m_B/m_F = 2.175$ or ^{40}K-^{87}Rb. The dashed lines are for the values of metastable states. The tiny window for phase separation near a_{cr} is too small to show here [see the inset of Fig. 3(a)].

asymptotically exact. And $a^{(1)}$, $a_{\rm cr}$ estimated in the limit of the large mass ratio ($k_F a^{(1)} \sim \pi/\ln[m_F/4m_B]$ in Fig. 3) are quantitatively valid. However, when $k_F a$ is of order 1, the fluctuations become substantial and the bound states can be further dressed in fluctuating particle-hole pairs; the energetic analyses are subject to corrections. To clarify this, we estimate the dominating effects of Fermi surface dynamics, i.e., the Gorkov-Melik-Barkhudarov (GMB) corrections in the two-body scattering vertex due to fluctuating particle-hole pairs [22,26,27], and the self-energy (SE) effect which mainly represents atomic Fermi surface smearing and the mass renormalization due to scattering by the condensate or Fermi sea. We then examine the pole structure of the propagator for a pair of Fermi-Bose atoms, taking into account these corrections, and we obtain the binding energy ω_B. The relative shift caused by the GMB effect (the leading order term R_1) and the SE effect (the higher order term R_2) is given as

$$\frac{\delta \ln|\omega_B|}{\ln|\omega_B|} = R_1(k_F a_{\rm bf}) + R_2(k_F a_{\rm bf})^2 \ln|k_F a_{\rm bf}| \ldots, \quad (7)$$

where $R_{1,2}$ are both dimensionless quantities depending on the mass ratio m_B/m_F and can be obtained diagrammatically [28]. For large mass ratios (m_B/m_F), one finds that $R_1 \sim -\ln(m_B/m_F)/\pi$ and $R_2 \sim -2/(3\pi^2)$, and ω_B is reduced by a factor of m_F/m_B solely due to the GMB effect. The net reduction in the binding energy ω_B leads to an upward shift of $1/a^{(1)}$ (dashed-dotted line) in Fig. 3. In addition, we have estimated that, for the paired state, the amplitude of pair fluctuations $A_1 \sim (\Delta/\epsilon_F^R)^4\sqrt{\kappa/m_R k_F}$ (κ is the compressibility of the paired mixture), and the corresponding zero point energy (in units of ϵ_F^R) per particle $A_2 \sim (\Delta/\epsilon_F^R)^4\sqrt{m_R k_F/\kappa}$. We incorporate these quantum fluctuations (analogous to NSR effects [11]) and the GMB correction into our analysis of the energetics of the paired state. For ^{40}K-^{87}Rb mixtures, we find that $A_1 \approx 0.01$, $A_2 \approx 0.003$ and $R_1 \approx -0.4$, $R_2 \approx -0.1$; the GMB and SE effects appear to be more dominant. The modified critical lines obtained by extrapolating the above analyses to near resonance are shown in Fig. 3 and are qualitatively consistent with the mean-field ones. The data suggest that quantum fluctuations tend to enlarge the window between $1/a_{\rm cr}$ and $1/a^{(1)}$ and further stabilize the first order phase transition. Quantum Monte Carlo simulations similar to those in Ref. [29] still need to be carried out.

In conclusion, we have examined dressed bound states and provided evidence of a new quantum state of extended molecules near broad interspecies resonances. As long as three- and higher-body correlations are insignificant, our results can be applied to understand Fermi-Bose mixtures near broad resonances.

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Note added.—Upon submission of this work, we learned that finite-temperature mixtures near broad resonances were studied in Ref. [30]. After acceptance of this Letter, we further learned the dimer dispersion was also discussed in Ref. [31].

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