Strongly Interacting Bose-Fermi Mixtures: Mediated Interaction, Phase Diagram, and Sound Propagation

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Motivated by recent surprising experimental findings, we develop a strong-coupling theory for Bose-Fermi mixtures capable of treating resonant interspecies interactions while satisfying the compressibility sum rule. We show that the mixture can be stable at large interaction strengths close to resonance, in agreement with the experiment, but at odds with the widely used perturbation theory. We also calculate the sound velocity of the Bose gas in the ^{133}Cs-^{6}Li mixture, again finding good agreement with the experimental observations both at weak and strong interactions. A central ingredient of our theory is the generalization of a fermion mediated interaction to strong Bose-Fermi scatterings and to finite frequencies. This further leads to a predicted hybridization of the sound modes of the Bose and Fermi gases, which can be directly observed using Bragg spectroscopy.

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Introduction.—The interest in mixtures of bosonic and fermionic quantum fluids has long predated the discovery of ultracold atomic gases. Indeed, as early as in the 1960s ^{3}He-^{4}He solutions were studied by London *et al.* [1], which led to the creation of an indispensable workhorse of low-temperature experiments—the dilution refrigerator [2]. For ultracold atomic gases, the Bose-Fermi mixture is not only practically valuable for sympathetically cooling the Fermi gas [3,4], but also serves as a versatile platform for studying a variety of physics, including polarons [5,6], mediated interactions [7–15], unconventional pairing [16,17], and dual superfluidity [18–20]. Because of its importance, more than a dozen different Bose-Fermi mixtures have so far been realized and studied experimentally (see Ref. [21] for a review).

Since the interspecies interaction can be tuned in an atomic Bose-Fermi mixture, the first fundamental question concerns its stability and miscibility [22–37]. For a weakly interacting Bose-Einstein condensate (BEC) mixed with a single-component Fermi gas, perturbation theory predicts that a sufficiently large Bose-Fermi scattering length will lead to the collapse of the system on the attractive side and to phase separation on the repulsive side [22–31]. At typical atomic gas densities, the predicted critical values of the scattering length are quite small such that perturbation theory is expected to be valid. The recent experimental results for the ^{133}Cs-^{6}Li mixture have therefore come as a surprise [38]. By measuring the bosonic sound propagation at varying Bose-Fermi scattering lengths, the experiments found that the mixture regains its stability near the interspecies Feshbach resonance, in contradiction with the perturbation theory [38].

In order to understand this puzzling phenomenon and more broadly the properties of resonant Bose-Fermi mixtures, we develop a strong-coupling approach based on the many-body Bose-Fermi scattering matrix. Importantly, our theory satisfies the compressibility sum rule [39], which plays a crucial role in determining the stability of the mixture. With this approach, we first obtain the zero-temperature phase diagram of the mixture corresponding to the experimental setup. The predicted region of stability is consistent with the experimental observation but differs significantly from that of the perturbative theory near resonance. An integral part of our theory is a generalization of the well-known Ruderman-Kittel-Kasuya-Yosida (RKKY) fermion mediated interaction [40] to the regime of strong Bose-Fermi scattering. Based on this interaction, we further calculate the speed of sound in the BEC and find reasonable agreement with the recent experiment for all interaction strengths. Finally, we show that the retarded nature of this mediated interaction leads to an intriguing hybridization of the BEC sound mode and an induced fermionic zero sound mode, which can be observed by Bragg spectroscopy.

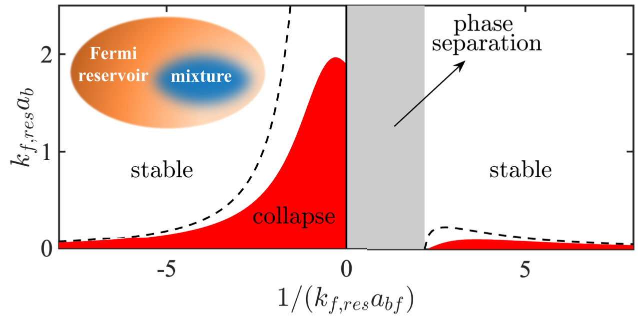

FIG. 1. Adiabatic phase diagram of the ^{133}Cs-^{6}Li mixture with density ratio $n_b/n_{f,\mathrm{res}} = 10$, where $n_{f,\mathrm{res}}$ is the reservoir fermion density and $k_{f,\mathrm{res}} \equiv (6\pi^2 n_{f,\mathrm{res}})^{1/3}$ is the corresponding Fermi momentum. The dashed lines are the stability boundaries calculated by the perturbation theory.

Bose-Fermi mixture.—We consider a mixture of a weakly interacting BEC of bosons with mass m_b and a noninteracting gas of fermions with mass m_f at zero temperature and in a configuration that is representative of many current experimental systems [14,15,38]. Namely, the BEC is completely immersed in a spatially much larger Fermi gas such that the Fermi gas surrounding the bosons acts effectively as a reservoir for the Fermi gas inside the mixture; this is illustrated in the inset of Fig. 1. The Hamiltonian for the mixture is

$$\hat{H} = \sum_{\boldsymbol{p}\neq 0}\left[(\epsilon_{b,\boldsymbol{p}} + 2g_b n_b)\hat{b}^\dagger_{\boldsymbol{p}}\hat{b}_{\boldsymbol{p}} + \frac{1}{2}g_b n_b(\hat{b}^\dagger_{\boldsymbol{p}}\hat{b}^\dagger_{-\boldsymbol{p}} + \mathrm{H.c.})\right] + \sum_{\boldsymbol{p}}\epsilon_{f,\boldsymbol{p}}\hat{f}^\dagger_{\boldsymbol{p}}\hat{f}_{\boldsymbol{p}} + g_{bf}\sum_{\boldsymbol{p}\boldsymbol{p}'\boldsymbol{q}}\hat{f}^\dagger_{\boldsymbol{p}}\hat{b}^\dagger_{\boldsymbol{p}'}\hat{b}_{\boldsymbol{p}'+\boldsymbol{q}}\hat{f}_{\boldsymbol{p}-\boldsymbol{q}}, \quad (1)$$

where $\hat{b}^\dagger_{\boldsymbol{p}}(\hat{f}^\dagger_{\boldsymbol{p}})$ creates a boson (fermion) of momentum $\boldsymbol{p}$ and energy $\epsilon_{i,\boldsymbol{p}} = \boldsymbol{p}^2/2m_i$ with $i = b(f)$. We have used the Bogoliubov theory to describe the BEC with density n_b and interaction strength $g_b = 4\pi a_b/m_b$, where a_b is the bosonic scattering length. The interspecies interaction strength g_{bf} is related to the Bose-Fermi scattering length in the usual way of $2\pi a_{bf}/m_r = g_{bf}/[1 + g_{bf}\int d^3\boldsymbol{k}(2\pi)^{-3}2m_r/k^2]$, where $m_r = m_b m_f/(m_b + m_f)$ is the reduced mass. Here we use units where $\hbar$ and the system volume are unity.

Strong-coupling theory.—In order to describe strong Bose-Fermi interactions, we use a Green's function approach with the Bose-Fermi scattering matrix as a basic building block [41–45]. Within this framework, the fermionic Green's function is given by [see Fig. 2(a)],

$$G_f(p) = \frac{1}{i\omega_p - (\epsilon_{f,\boldsymbol{p}} - \mu_f) - n_b\mathcal{T}_{bf}(p)}, \quad (2)$$

where μ_f is the chemical potential of the fermions inside the mixture, ω_p is the Matsubara frequency, and $p \equiv (i\omega_p, \boldsymbol{p})$. The scattering matrix between a boson and a Fermi gas of

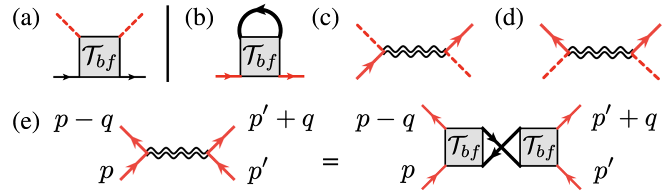

FIG. 2. Self-energy diagrams for (a) fermions and (b)–(d) bosons due to the Bose-Fermi interaction. The (dashed) red line denotes a (condensate) boson and the black line a fermion. The wavy line denotes the fermion mediated interaction in Eq. (6), which is described by the Feynman diagram in (e).

density n_f is

$$\mathcal{T}_{bf}(p) = \frac{1}{m_r/2\pi a_{bf} - \Pi_{bf}(p)}, \quad (3)$$

with the pair propagator

$$\Pi_{bf}(p) = \int\frac{d^3\boldsymbol{k}}{(2\pi)^3}\left[\frac{1 - n_{\mathrm{FD}}(\boldsymbol{k})}{i\omega_p - \epsilon_{b,\boldsymbol{p}-\boldsymbol{k}} - \xi_{f,\boldsymbol{k}}} + \frac{2m_r}{k^2}\right]. \quad (4)$$

Here $\xi_{f,\boldsymbol{k}} = \boldsymbol{k}^2/2m_f - k_f^2/2m_f$ with $k_f \equiv (6\pi^2 n_f)^{1/3}$ and $n_{\mathrm{FD}}(\boldsymbol{k}) = \theta(\xi_{f,\boldsymbol{k}})$ is the Fermi-Dirac distribution. We have neglected the effects of the BEC on the pair propagator in Eq. (4) and therefore the dependence of the fermion density n_f on the Bose scattering length a_b, which is a good approximation for weakly interacting Bose gases with $n_b a_b^3 \ll 1$ [46].

To the lowest order in the scattering matrix, the effects of the Fermi gas on the BEC are captured by the self-energy diagram shown in Fig. 2(b). As shown in the Supplemental Material [47], in order to fulfill the compressibility sum rule, one also needs to include the diagrams in Figs. 2(c) and 2(d), which are second order in $\mathcal{T}_{bf}$. Incorporating also the usual Bogoliubov self-energies due to the weak boson-boson scattering, we find

$$\Sigma_{11}(p) = 2n_b g_b + \sum_k G_f(k)\mathcal{T}_{bf}(k+p) + n_b\Gamma_{\mathrm{MI}}(p, 0; p),$$
$$\Sigma_{12}(p) = n_b g_b + n_b\Gamma_{\mathrm{MI}}(p, -p; p) \quad (5)$$

as the normal and anomalous self-energies of the BEC. Here we have defined the generalized fermion mediated interaction [shown in Fig. 2(e)],

$$\Gamma_{\mathrm{MI}}(p, p'; q) = \sum_k G_f(k)G_f(k+q) \times \mathcal{T}_{bf}(p+k)\mathcal{T}_{bf}(p'+k+q), \quad (6)$$

where $\sum_k \equiv T\sum_{i\omega_k}\int[d^3\boldsymbol{k}/(2\pi)^3]$ with temperature T. The normal and anomalous Green's functions of the BEC can be obtained from the coupled equations [48,49]

$$[G^0(p)^{-1} - \Sigma_{11}(p)]G_{11}(p) - \Sigma_{12}(p)G_{12}(p) = 1; \quad (7)$$

$$[G^0(-p)^{-1} - \Sigma_{11}(-p)]G_{12}(p) - \Sigma_{12}(p)G_{11}(p) = 0, \quad (8)$$

where $G^0(p) = (i\omega_p - \epsilon_{b,\boldsymbol{p}} + \mu_b)^{-1}$ and μ_b is the bosonic chemical potential. To ensure that the bosonic spectrum is gapless, the chemical potential must satisfy the Hugenholtz-Pines theorem $\mu_b = \Sigma_{11}(0) - \Sigma_{12}(0)$ [48]. From Eq. (5), we find

$$\mu_b = n_b g_b + \sum_k G_f(k)\mathcal{T}_{bf}(k). \quad (9)$$

Solving Eqs. (7)–(9) yields the bosonic Green's functions, which can be used to calculate the Bogoliubov spectrum $E_{b,\boldsymbol{p}}$ and other physical properties. We emphasize that we focus on mixtures in which the condensate depletion due to the Bose-Fermi scattering is negligible even in the strong-coupling regime [47].

Adiabatic phase diagram.—We first use our strong-coupling theory to construct the zero-temperature adiabatic phase diagram spanned by the two scattering lengths a_b and a_{bf}. The stability and miscibility of the mixture are determined by two conditions [50]: (a) the chemical potential μ_f of the Fermi gas within the mixture equals that of the reservoir $\mu_{f,\mathrm{res}}$; (b) the compressibility of the BEC under a fixed fermion chemical potential is positive definite [51], i.e., $(\partial\mu_b/\partial n_b)|_{\mu_f} \geq 0$. The first condition places a constraint on the fermion density inside the mixture, while the second ensures that the mixture is stable against collapse. In Fig. 1, we show the phase diagram obtained from these conditions for the experimentally relevant case of a ^{133}Cs-^{6}Li mixture with density ratio $n_b/n_{f,\mathrm{res}} = 10$, where the reservoir density is $n_{f,\mathrm{res}} = k_{f,\mathrm{res}}^3/6\pi^2$ with $k_{f,\mathrm{res}} \equiv \sqrt{2m_f\mu_{f,\mathrm{res}}}$. We now discuss in detail how this phase diagram is obtained.

Using the condition $\mu_f = \mu_{f,\mathrm{res}}$, the fermionic quasiparticle dispersion $\varepsilon_{f,\boldsymbol{p}}$ is determined from the poles of $G_f(p)$ and the fermion density inside the mixture is calculated as $n_f = \sum_p G_f(p)$. We find that, similar to the so-called Bose polaron, i.e., a single fermion in a BEC [52–54], the fermionic Green's function also has two quasiparticle branches: an attractive and a repulsive one; the attractive (repulsive) branch has negative (positive) energy and takes most of the spectral weight for $a_{bf} < 0$ ($a_{bf} > 0$). These two branches are shown in Fig. 3(a) for the ^{133}Cs-^{6}Li mixture. Hence, we assume that the fermions occupy the attractive branch for $a_{bf} < 0$ and the repulsive branch for $a_{bf} > 0$. This corresponds to scenarios where the mixture is initially prepared at weak Bose-Fermi interactions on either side of the resonance and is then adiabatically ramped toward the resonance by tuning a_{bf} infinitely slowly. Since μ_f is fixed by the reservoir, it follows that the density n_f of fermions occupying the attractive branch increases as a_{bf} is tuned from a small negative value to resonance; the opposite is true for fermions occupying the repulsive branch. This is shown in Fig. 3(b). Thus, in the latter case, the fermion density inside the mixture vanishes beyond a critical value of a_{bf} as the fermions in the repulsive branch are eventually all repelled from the mixture, leading to phase separation between the fermions and the bosons indicated by the gray region in Fig. 1.

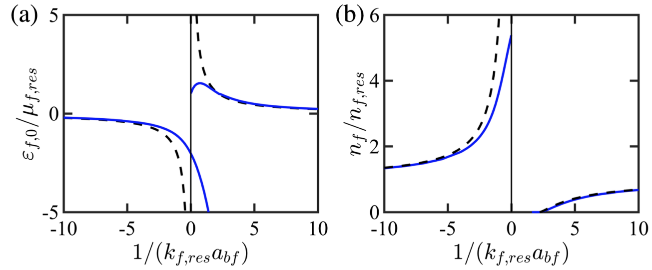

FIG. 3. (a) The attractive and repulsive fermion quasiparticle branch $\varepsilon_{f,\boldsymbol{p}=0}$ for the ^{133}Cs-^{6}Li mixture of Fig. 1. (b) Corresponding fermion densities inside the mixture. Solid and dashed lines are the strong-coupling and perturbation theory, respectively. We assume for the moment that the mixture is always stable.

Outside the region of phase separation, the stability of the mixture is determined by the compressibility of the BEC. From Eq. (9), we find

$$\left.\frac{\partial\mu_b}{\partial n_b}\right|_{\mu_f} = \frac{4\pi}{m_b}\left[a_b + \frac{m_b}{4\pi}\Gamma_{\mathrm{MI}}(0,0;0)\right]. \quad (10)$$

This relation naturally leads to an effective scattering length from the fermion mediated interaction given by

$$a_{\mathrm{eff}} \equiv \frac{m_b}{4\pi}\Gamma_{\mathrm{MI}}(0,0;0). \quad (11)$$

It then follows from Eq. (10) that the BEC collapses when the total scattering length $a_b + a_{\mathrm{eff}}$ turns negative.

In the weak Bose-Fermi interaction limit, we can replace $\mathcal{T}_{bf}$ by $2\pi a_{bf}/m_r$ and the fermion mediated interaction in Eq. (6) reduces to the familiar RKKY form $\Gamma_{\mathrm{MI}}(q) = (4\pi^2 a_{bf}^2/m_r^2)\chi_f^{(0)}(i\omega_q, \boldsymbol{q})$ [10,11], where $\chi_f^{(0)}(i\omega_q, \boldsymbol{q})$ is the Lindhard function of a free Fermi gas. Since $\chi_f^{(0)}(0,\boldsymbol{q}) = -(m_f k_f/2\pi^2)(1 - q^2/8k_f^2)$ in the long wavelength limit, second order perturbation theory predicts that $a_{\mathrm{eff}} = -(1/2\pi)(m_f/m_b + m_b/m_f + 2)k_f a_{bf}^2$ [38,47]. In Fig. 4 we compare this result against that calculated by our strong-coupling theory. We find that, while the two approaches agree for weak coupling as expected, the strong-coupling result for a_{eff} is significantly smaller close to unitarity. Qualitatively similar behavior of the effective scattering length was also found using the Born-Oppenheimer approximation in the absence of a BEC [55].

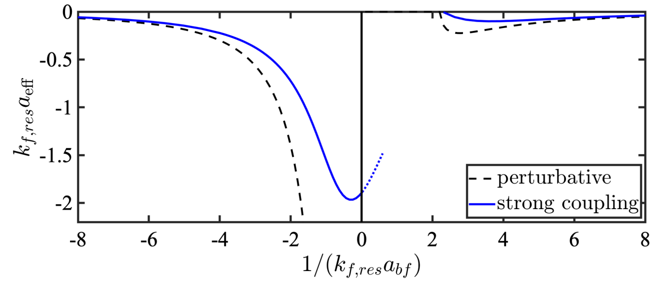

FIG. 4. The effective scattering lengths from the mediated interaction, calculated by the perturbation theory and the strong-coupling theory. The blue dotted line shows the behavior of $a_{\rm eff}$ assuming the fermions stay on the attractive branch beyond the resonance. The results are for the ^{133}Cs-^{6}Li mixture of Fig. 1.

This has important consequences for the phase diagram. Since the BEC collapses for $a_b + a_{\rm eff} < 0$ as discussed above, the values of $a_{\rm eff}$ shown in Fig. 4 directly give the boundaries for the collapse regions shown in Fig. 1. While perturbation theory predicts a collapse region that extends to arbitrarily large values of a_b as unitarity $1/a_{bf} = 0$ is approached, our strong-coupling theory predicts a much smaller collapse region bounded by a maximum value of a_b near resonance. It follows that the mixture is stable even at resonance provided that a_b is sufficiently large. In Fig. 1, we see that the region of stability of the Bose-Fermi mixture, indeed, is significantly larger than that predicted from the perturbation theory.

Bosonic sound propagation.—We next turn to the discussion of bosonic sound propagation observed recently in a strongly interacting ^{133}Cs-^{6}Li mixture [38]. As usual, the Bogoliubov sound velocity in the BEC is defined from the Bogoliubov spectrum as $c_b = \lim_{\boldsymbol{p}\to 0} E_{b,\boldsymbol{p}}/|\boldsymbol{p}|$. In a pure BEC, this velocity is given by $c_b^{(0)} = \sqrt{n_b g_b/m_b}$, which coincides with that defined by the compressibility $c_{b,\rm com} = \sqrt{(n_b/m_b)\partial\mu_b/\partial n_b}$ [39]. Interestingly, these two quantities are not equal in the Bose-Fermi mixture due to the retarded nature of the fermion mediated interaction. Retardation effects can, however, be ignored when the Fermi velocity v_f is much larger than the sound velocity in the pure BEC, i.e., when $c_b^{(0)}/v_f = (m_f/m_b)\sqrt{(2/3\pi)(n_b/n_f)(k_f a_b)} \ll 1$. This is indeed the case for the ^{133}Cs-^{6}Li mixture in Ref. [38] due to the very small Fermi-Bose mass ratio.

We therefore use the compressibility formula to calculate the sound velocity and compare the results with the recent experiment. In order to do so, we first note an important difference between the physical scenario addressed by the thermal equilibrium phase diagram and that by the experimental situation. As mentioned earlier, the phase diagram corresponds to assuming an adiabatic ramping from weak Bose-Fermi interactions to the relevant a_{bf}. In contrast, the mixture in Ref. [38] is prepared at a small a_{bf} and is then ramped to any target value of a_{bf} within a fixed duration of time. Thus, the experimental process is approximately adiabatic only for small target values a_{bf}, but highly nonadiabatic for target values in the resonant regime. Consequently, a significant fraction of the fermions will not remain on the same quasiparticle branch under such nonadiabatic ramps due to Landau-Zener transitions [56,57]. Furthermore, heavy losses of atoms are also observed in experiments near resonance [38]. For these reasons, one must expect that near resonance the experimental values for the fermion densities inside the mixture will deviate significantly from those predicted by our thermal equilibrium theory described above. In particular, if the ramping is from the repulsive to the attractive side, then a portion of fermions will transition from the repulsive to the attractive branch in the resonant regime and thus remain in the mixture to affect the sound propagation of the Bose gas; if the ramping is along the opposite direction, on the other hand, a portion of fermions will transition from the attractive to the repulsive branch in the resonant regime and are thus repelled from mixture, leading to a smaller fermion density. Indeed, using the experimental parameters $n_b \approx 1.87\times 10^{19}\ {\rm m}^{-3}$, $n_{f,\rm res} \approx 3\times 10^{17}\ {\rm m}^{-3}$, and $a_b = 270 a_0$, where a_0 is the Bohr radius, the adiabatic phase diagram corresponding to $n_b/n_{f,\rm res} \approx 60$ predicts collapse and phase separation at $1/k_{f,\rm res}a_{bf} \simeq -11.5$ and $1/k_{f,\rm res}a_{bf} \simeq 13$, respectively. However, a well-defined sound mode is observed in the resonant region, which we attribute to the nonequilibrium effects described above. To make comparisons with experiments conducted near resonant a_{bf}, we therefore treat n_f as a fitting parameter using $n_f/n_{f,\rm res} = 0.006 + 0.05(k_{f,\rm res}a_{bf})^{-1/2}$ for $0 < 1/k_{f,\rm res}a_{bf} \lesssim 8$ and $n_f/n_{f,\rm res} = 0.006 - 0.0002(k_{f,\rm res}a_{bf})^{-3}$ for $-3 \lesssim 1/k_{f,\rm res}a_{bf} < 0$ as suggested by the observed loss in the experiments [38]. First, we see from Fig. 5 that, in the regime where thermal equilibrium theory can be applied, both perturbative and strong-coupling theories with no fitting of n_f agree well with experiment. Our strong-coupling theory has a slightly better agreement, particularly on the attractive side close to collapse where the sound

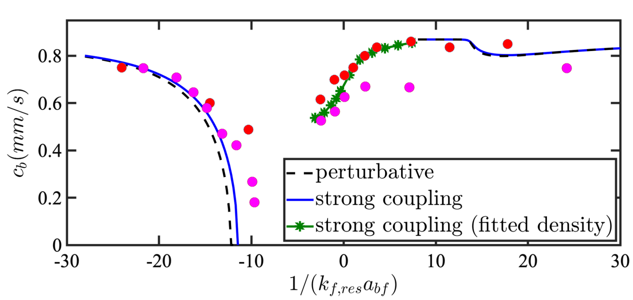

FIG. 5. Comparison of our strong-coupling theory for the BEC sound velocity to the experimental results (dots) in Ref. [38]. The dots in magenta (red) are data obtained from a ramping procedure that begins at the attractive (repulsive) side and ends at the repulsive (attractive) side.

velocity goes to zero, as also seen experimentally. The kink in the theoretical curve at $1/k_{f,\mathrm{res}}a_{bf} \simeq 13$ is due to phase separation, causing the sound velocity to return to that of a pure BEC. Second, for resonant a_{bf} perturbative theory predicts no sound propagation, while the strong-coupling theory with fitted n_f reproduces the experimental measurements well.

Retardation and induced fermionic zero sound.—The Fermi-Bose mass ratio is much larger for a ^{23}Na-^{40}K mixture [58–61] compared to a ^{133}Cs-^{6}Li mixture, and it follows from the arguments given above that retardation effects can be significant for the former. A remarkable consequence of this is the possibility of exciting an induced fermionic zero sound mode through a bosonic density perturbation. It is known that in a Bose-Fermi mixture the noninteracting fermions can also experience a mediated interaction due to the Bose gas, which can lead to a fermionic zero sound mode with a speed $\sim v_f$ [62–64]. When the Bose-Fermi interaction is strong and the zero sound velocity is comparable to that in the pure BEC, we anticipate a strong coupling of these two modes.

In order to demonstrate this, we turn to the calculation of the dynamic structure factor of the BEC, which also gives the sound spectrum [39] and can be directly probed by Bragg spectroscopy [65,66]. It is defined as

$$S_b(\omega,\boldsymbol{p}) \equiv \frac{1}{\pi}\mathrm{Im}\chi_b(i\omega_p \to \omega + i0^+,\boldsymbol{p}). \qquad (12)$$

Here $\chi_b(p)$ is the density-density response function of the BEC and is given by $\chi_b(p) = -2N_b[G_{11}(p) + G_{11}(-p) + 2G_{12}(p)]$ within the Bogoliubov framework, where N_b is the total number of bosons. We now calculate $S_b(\omega,\boldsymbol{p})$ for a strongly interacting ^{23}Na-^{40}K mixture with $n_b/n_f = 10$, $k_f a_b = 0.067$, and $1/(k_f a_{bf}) = -3$, which yields $c_b^{(0)}/v_f \sim 0.65$. As shown in Fig. 6(a), $S_b(\omega,\boldsymbol{p})$ exhibits a double peak structure, indicating the presence of two modes, in stark contrast with the single peak structure at small a_{bf} or for $c_b^{(0)}/v_f \ll 1$ (Supplemental Material [47]). Figure 6(b) plots the dispersion of these two modes, which are compared to the single mode in a pure BEC. This explicitly demonstrates that a fermionic zero sound mode indeed can hybridize with the Bogoliubov sound mode and manifest itself in the excitation spectrum of the BEC.

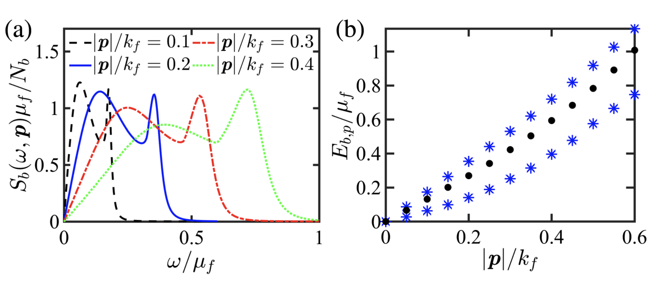

FIG. 6. (a) Dynamic structure factor $S_b(\omega,\boldsymbol{p})$ of the BEC at different momenta for a strongly interacting ^{23}Na-^{40}K mixture. (b) Excitation spectrum $E_{b,\boldsymbol{p}}$ obtained from the peaks of $S_b(\omega,\boldsymbol{p})$ (blue asterisks) and for a pure BEC (black dots).

Concluding remarks.—We have developed a strong-coupling theory for the ground state and collective excitations of strongly interacting Bose-Fermi mixtures, emphasizing the role of a generalized mediated interaction. Our theory agrees well with recent experimental results for a resonant ^{133}Cs-^{6}Li mixture, for which the much used perturbation theory fails to account. Furthermore, we show that new, interesting physics caused by retardation of the generalized mediated interaction can be revealed by the bosonic dynamic structure factor and observed in future experiments. Finally, in light of many different mixtures being studied experimentally, our approach may be used to systematically explore effects of mass and density ratio on properties of strongly interacting Bose-Fermi mixtures.

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