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Bose polarons at finite temperature and strong coupling

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A mobile impurity coupled to a weakly-interacting Bose gas, a Bose polaron, displays several interesting effects. While a single attractive quasiparticle is known to exist at zero temperature, we show here that the spectrum splits into two quasiparticles at finite temperatures for sufficiently strong impurity-boson interaction. The ground state quasiparticle has minimum energy at T_c , the critical temperature for Bose-Einstein condensation, and it becomes overdamped when $T \gg T_c$. The quasiparticle with higher energy instead exists only below T_c , since it is a strong mixture of the impurity with thermally excited collective Bogoliubov modes. This phenomenology is not restricted to ultracold gases, but should occur whenever a mobile impurity is coupled to a medium featuring a gapless bosonic mode with a large population for finite temperature.

Mobile impurities in a quantum bath play a fundamental role in a wide range of systems including metals and dielectric materials [1], semiconductors [2], ^3He - ^4He mixtures [3], and high- T_c superconductors [4]. In certain limits, they provide a paradigmatic realization of Landau’s fundamental concept of a quasiparticle. The precise experimental measurements on impurity atoms in ultracold Fermi gases [5–9] combined with several theoretical investigations [10–18] led to fundamental insights into this problem. Recently, two experimental groups embedded impurity atoms in a Bose-Einstein condensate (BEC) and observed long-lived quasiparticles coined Bose polarons [19, 20]. Bose polarons have been investigated using a variety of theoretical techniques [21–32], and they have also been considered in one dimension [33–37].

A qualitatively new feature of the Bose polaron with respect to polarons in a Fermi gas or in solid state systems is that the environment undergoes a phase transition to a BEC at T_c . This changes drastically the low-energy density-of-states of the environment, and should therefore affect significantly the polaron. Temperature effects on Bose polarons have been examined so far only theoretically, either in the mean-field regime [38], at high temperature [39], or for immobile Rydberg atoms [30].

Here, we develop a strong coupling diagrammatic scheme designed to include scattering processes important for finite temperature. Using this, we show that the polaron splits into two quasiparticle states for $0 < T < T_c$ for strong attractive coupling. The energy of the lower polaron depends non-monotonically on temperature with a minimum at T_c , whereas the energy of the upper polaron increases until its quasiparticle residue vanishes at T_c . The generic mechanism causing these effects is the coupling between the impurity and low energy Bogoliubov modes with an infrared divergent population for finite T . Consequently, similar effects should occur whenever a mobile impurity is coupled to a gapless bosonic mode, as for example in Helium liquids or quantum mag-

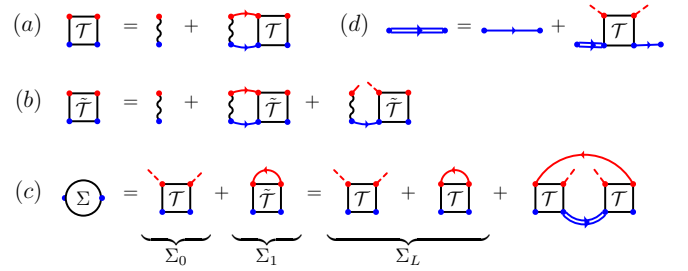


FIG. 1. Feynman diagrams yielding the self-energy Σ within the “extended” ladder approximation. Thin blue lines represent the bare impurity propagator, solid red lines are Bogoliubov propagators, dashed red lines are condensate bosons, and wavy lines represent the vacuum scattering matrix \mathcal{T}_v . The ladder self-energy is indicated by Σ_L , and the double blue line is an impurity dressed by the condensate only.

nets. Indeed, an analogous splitting has been predicted for quasiparticle modes in hot electron and quark-gluon plasmas [40–43], providing an interesting link between low and high energy quantum phenomena.

System.— We consider a single impurity particle of mass m , immersed in a gas of weakly-interacting bosons of mass m_B and density n at temperature T . We take $\hbar = k_B = 1$, and measure momenta and energies in units of $k_n = (6\pi^2 n)^{1/3}$ and $E_n = k_n^2/2m_B$. The boson-boson interaction is short-ranged and characterized by a scattering length a_B , and the condition of weak interaction means $0 < k_n a_B \ll 1$. Below the critical temperature $T_c = [4/(3\sqrt{\pi}\zeta(3/2))]^{2/3} E_n \approx 0.436 E_n$, the bosons are accurately described using Bogoliubov theory [44]. The condensate density is $n_0 = n[1 - (T/T_c)^{3/2}]$ and the chemical potential is $\mu_B = \mathcal{T}_B n_0$ with $\mathcal{T}_B = 4\pi a_B/m_B$. The dispersion of the excitations reads $E_{\mathbf{k}} = [\epsilon_{\mathbf{k}}^B(\epsilon_{\mathbf{k}}^B + 2\mu_B)]^{1/2}$, with $\epsilon_{\mathbf{k}}^B = k^2/2m_B$. Above T_c the condensate disappears, the excitations become free bosons, $E_{\mathbf{k}} = \epsilon_{\mathbf{k}}^B$, and the chemical potential reduces to that of an ideal Bose gas. The impurity interacts with the bath through

a short-ranged potential described by the s -wave scattering length a . Given that we study a single impurity, we consider its effect on the Bose cloud negligible.

Diagrammatic analysis.— An impurity with momentum \mathbf{k} is described by the imaginary-time Green's function $\mathcal{G}(\mathbf{k}, i\omega_j) = 1/[\mathcal{G}_0(\mathbf{k}, i\omega_j)^{-1} - \Sigma(\mathbf{k}, i\omega_j)]$, where $\mathcal{G}_0(\mathbf{k}, i\omega_j) = (i\omega_j - \epsilon_{\mathbf{k}})^{-1}$ with $\epsilon_{\mathbf{k}} = k^2/2m$ is the Green's function of a free impurity, and $\omega_j = 2\pi jT$ is a Matsubara frequency [44, 45]. The key quantity to calculate is the impurity self-energy $\Sigma(\mathbf{k}, i\omega_j)$, and in presence of strong interactions we must resort to suitable approximations. As a minimum, we have to include the ladder diagrams of Fig. 1(a), which describe the energy shift due to two-body processes between the impurity and Bogoliubov excitations. This yields the ladder scattering matrix $\mathcal{T}(\mathbf{p}, i\omega_j) = 1/[\mathcal{T}_v^{-1} - \Pi(\mathbf{p}, i\omega_j)]$, where $\mathcal{T}_v = 2\pi a/m_r$ is the vacuum scattering amplitude, $m_r = mm_B/(m + m_B)$ is the reduced mass, and $\Pi(\mathbf{p}, i\omega_j) = \int \frac{d^3k}{(2\pi)^3} \left(\frac{u_{\mathbf{k}}^2(1+f_{\mathbf{k}})}{i\omega_j - E_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{p}}} + \frac{v_{\mathbf{k}}^2 f_{\mathbf{k}}}{i\omega_j + E_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{p}}} + \frac{2m_r}{k^2} \right)$ is the renormalized pair propagator for an impurity and a boson from the bath. Here $f_{\mathbf{k}} = 1/[\exp(E_{\mathbf{k}}/T) - 1]$ is the Bose distribution, and $u_{\mathbf{k}}^2 = [(\epsilon_{\mathbf{k}}^B + \mu_B)/E_{\mathbf{k}} + 1]/2$ and $v_{\mathbf{k}}^2 = u_{\mathbf{k}}^2 - 1$ are the Bogoliubov coherence factors.

A very recent perturbative analysis [46] showed that events where the impurity scatters excited bosons into the BEC are important at finite temperatures. To include these events, which are not contained in the ladder approximation, we introduce the “extended” scattering matrix $\tilde{\mathcal{T}}$ shown in Fig. 1(b), and given by

$$\tilde{\mathcal{T}}(\mathbf{p}, i\omega_j) = \frac{1}{\mathcal{T}_v^{-1} - \Pi(\mathbf{p}, i\omega_j) - n_0 \mathcal{G}_0(\mathbf{p}, i\omega_j)}. \quad (1)$$

Compared to the ladder approximation \mathcal{T} , the denominator of $\tilde{\mathcal{T}}$ contains the additional term $n_0 \mathcal{G}_0(\mathbf{p}, i\omega_j)$, which describes pair propagation where the entire momentum is carried by the impurity while the boson is in the BEC. This process is represented by the third term in Fig. 1(b).

As shown in Fig. 1(c), within the extended scheme the impurity self-energy is $\Sigma = \Sigma_0 + \Sigma_1$, where

$$\Sigma_0(\mathbf{p}, i\omega_j) = n_0 \mathcal{T}(\mathbf{p}, i\omega_j) \quad (2)$$

is the energy shift experienced by the impurity through interactions with the condensate only, and

$$\Sigma_1(\mathbf{p}, i\omega_j) = \int \frac{d^3k}{(2\pi)^3} \left[u_{\mathbf{k}}^2 f_{\mathbf{k}} \tilde{\mathcal{T}}(\mathbf{k} + \mathbf{p}, i\omega_j + E_{\mathbf{k}}) + v_{\mathbf{k}}^2 (1 + f_{\mathbf{k}}) \tilde{\mathcal{T}}(\mathbf{k} + \mathbf{p}, i\omega_j - E_{\mathbf{k}}) \right] \quad (3)$$

is the energy shift coming from interactions with bosons excited out of the BEC. Note that replacing \mathcal{T} with $\tilde{\mathcal{T}}$ in Σ_0 is not allowed, since this would lead to double counting of diagrams. As shown in Fig. 1(c), Σ_1 may be decomposed in two contributions: one where the impurity scatters a boson from an excited state to another (second

diagram), and one where the excited bosons are scattered virtually back into the BEC (last diagram). An approximation similar to ours was used in Ref. [47] for analyzing Bose-Fermi mixtures, while the ladder approximation Σ_L (considered at $T = 0$ in Ref. [27]) is recovered by replacing $\tilde{\mathcal{T}}$ with \mathcal{T} in (3), which is equivalent to neglecting the rightmost diagram in Fig. 1(c).

The spectral function of the impurity particle with momentum \mathbf{p} is given by $A(\mathbf{p}, \omega) = -2\text{Im}[G(\mathbf{p}, \omega)]$, where we have performed the usual analytic continuation $i\omega_j \rightarrow \omega + i0_+$, suppressing $i0_+$ for notational simplicity. A quasiparticle corresponds to a sharp peak in the spectral function. Its energy is found by solving

$$\omega_{\mathbf{p}} = \epsilon_{\mathbf{p}} + \text{Re}[\Sigma(\mathbf{p}, \omega_{\mathbf{p}})], \quad (4)$$

and the quasi-particle is well-defined when the damping $\Gamma = -Z_{\mathbf{p}} \text{Im}[\Sigma(\mathbf{p}, \omega_{\mathbf{p}})]$ is small. Here $Z_{\mathbf{p}} = 1/\{1 - \partial_{\omega} \text{Re}[\Sigma(\mathbf{p}, \omega)]|_{\omega_{\mathbf{p}}}\}$ is the residue, a measure for the spectral weight of the quasiparticle peak.

Results.— We now show numerical results for the properties of the dressed impurity, taking for concreteness equal impurity and boson masses $m = m_B$ corresponding to the Aarhus experiment [19]. Having this experiment in mind, we also focus on zero momentum polarons. Unless otherwise specified, we set $k_n a_B = 0.01$.

The impurity spectral function is shown in Fig. 2 as a function of temperature for $k_n a = -1$. We plot results obtained from both the extended scheme and the ladder approximation. For $T = 0$, the two schemes give essentially the same result: The spectral function exhibits a single narrow peak corresponding to a quasiparticle, the attractive polaron, with energy $\omega \simeq -0.3E_n$. This is not surprising, since $k_n a_B = 0.01 \ll 1$ and very few bosons are excited out of the BEC at $T = 0$, so that Σ_1 is negligible in both the ladder and the extended scheme.

Significant differences between the two approximations appear however for $T > 0$. As shown in Fig. 2, while the spectral function in the ladder approximation exhibits a single polaron peak, corresponding to a single quasiparticle solution of ω_L of (4), the extended approximation yields *two quasiparticle peaks* in the spectral function. Correspondingly, there are *two* quasiparticle (polaron) solutions to (4), ω_{\uparrow} and ω_{\downarrow} . Just above $T = 0$, the two sharp polaron peaks emerge symmetrically out of the ladder polaron with similar spectral weight. In fact, their residues Z_{\uparrow} and Z_{\downarrow} are both close to $Z_L/2$. Both features can be explained by a pole expansion valid for $k_n a_B \ll 1$ [48]. For weak coupling, $\omega_{\uparrow, \downarrow} \simeq \omega_0(1 \pm \sqrt{Z_0 n_{\text{ex}}/n_0})$, where $\omega_0 = n_0 \mathcal{T}_v$ is the energy of a zero momentum impurity dressed by the condensate only, and $n_{\text{ex}} = n - n_0(T)$ is the density of bosons excited out of the condensate [48]. The energy of the upper polaron ω_{\uparrow} increases with T , but its spectral weight drops to zero as T_c is approached. The energy of the lower polaron ω_{\downarrow} instead decreases with temperature, reaching a minimum at T_c , after which it increases. For $T \geq T_c$

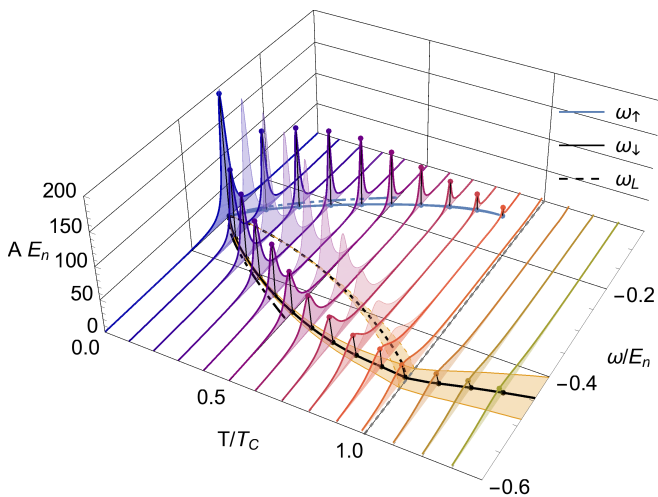


FIG. 2. Spectral function $A(\omega)$ of the attractive polarons (in units of $1/E_n$) versus T at $k_n a_B = 0.01$ and $k_n a = -1$, computed using the ladder approximation (dashed lines and lighter shading) and our extended model (thick lines and darker shading). For clarity, we added an artificial tiny width of $0.01E_n$ to the spectral lines. The thick solid lines in the plane show the polaron energies, as given by Eq. (4), and the width of their shading gives the damping Γ . The dash-dotted lines are the low temperature result $\omega_0(1 \pm \sqrt{Z_0 n_{ex}/n_0})$.

there is no BEC, and the extended and ladder approximation coincide. The width of the lower polaron peak increases with temperature reflecting increased damping due to scattering on thermally excited bosons. Eventually, the polaron becomes ill-defined for $T \gg T_c$.

In Fig. 3, we show the quasiparticle spectrum and residues at unitarity $1/k_n a = 0$, obtained by solving (4). This shows the same physics as we found for $k_n a = -1$, but scaled to larger binding energies. Using a virial expansion to compute the self-energy for $T \gg T_c$, and assuming also $T \gg 1/m_r a^2$, we obtain

$$\Sigma(0,0) \approx -i \frac{4E_n}{3\pi^{3/2}} \left(\frac{m_B}{m_r}\right)^2 \sqrt{\frac{E_n}{T}}. \quad (5)$$

Thus, at high temperature the polaron energy approaches zero, and the quasiparticle becomes overdamped. Our numerical results converge to (5) for $T \gg T_c$, although such high temperatures are not shown in Figs. 2 and 3.

In Fig. 4 we plot the energy of the attractive polaron as a function of the interaction strength $1/k_n a$, for $k_n a_B = 0.01$ and at various temperatures. For all coupling strengths $a \gtrsim a_B$, we observe that the single attractive polaron present at $T = 0$ splits into two polarons at intermediate temperatures, of which only the lower one survives at $T \geq T_c$.

To analyze the origin of the splitting, in Fig. 5 we plot $\text{Re}[\Sigma(\omega)]$ for $k_n a = -0.1$ and various values of $k_n a_B$ and T/T_c . Graphically, the quasiparticle solutions (4) are determined by the crossing of $\text{Re}[\Sigma(\omega)]$ with the diagonal

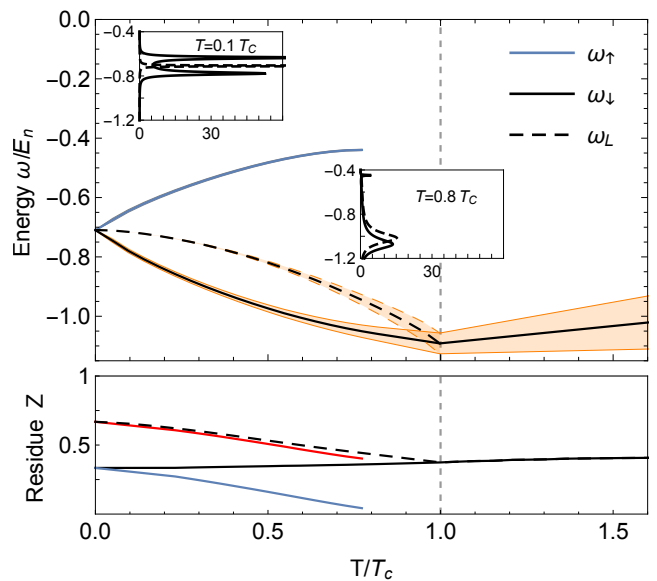


FIG. 3. Energies (top) and residues (bottom) of the attractive polarons for $1/k_n a = 0$ in the ladder approximation (dashed line) and from our extended model (solid lines). The width of the shading around the energies gives the damping Γ . We stop plotting ω_\uparrow when its residue is below 5%. The insets depict the spectral function $A(\omega)$ at $T = 0.1T_c$ (left) and $T = 0.8T_c$ (right). The red line shows $Z_\uparrow + Z_\downarrow$.

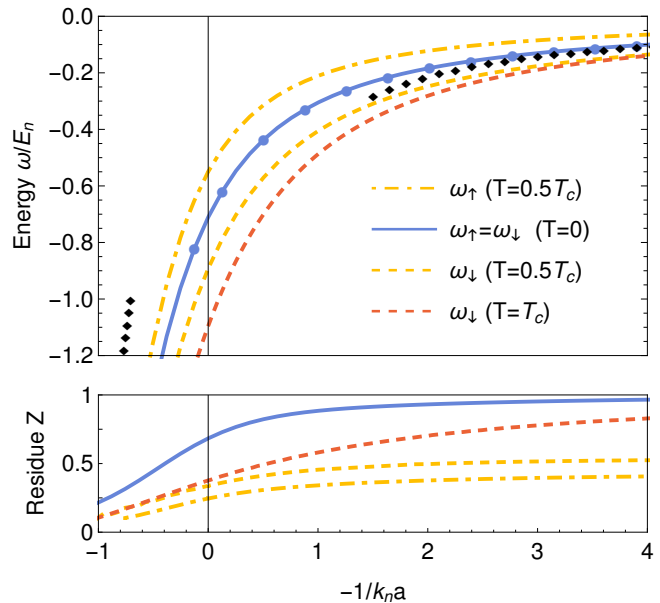


FIG. 4. Energy (top) and residue (bottom) of the attractive polarons versus interaction strength, at $T = 0$ (blue), $T = 0.5T_c$ (yellow), and $T = T_c$ (red). The filled blue circles in the energy plot indicate the results of the ladder approximation at $T = 0$, and the two black lines (filled diamonds) are the mean field results $\omega = 2\pi a/m_r$ (right) and $\omega = -1/(2m_r a^2) + \mu_B$ (left), valid respectively for $-1/k_n a \gg 1$ and $-1/k_n a \ll -1$.

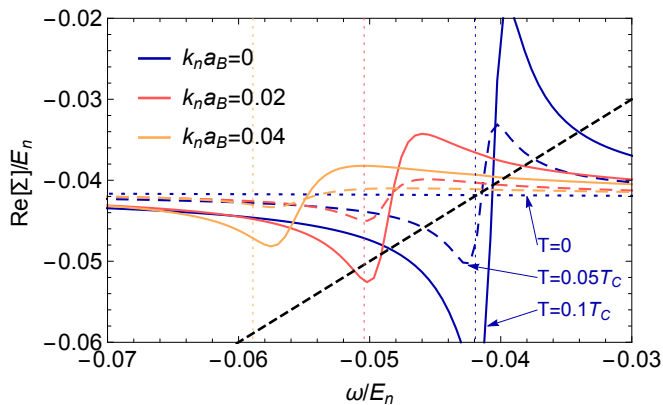


FIG. 5. Real part of the self-energy $\Sigma(\mathbf{p} = 0, \omega)$ for $k_n a = -0.1$, at $T = 0$ (purple dotted line, almost horizontal), $T = 0.05T_c$ (dashed) and $T = 0.1T_c$ (solid). The different colors correspond to various values of $k_n a_B$. The diagonal black line represents ω , and the vertical lines denote $n_0(\mathcal{T}_v - \mathcal{T}_B)$.

dashed line giving ω . Focus first on the purple lines relevant for a very small value of $k_n a_B$. For $T = 0$ (purple dotted line, almost horizontal) there is only one solution close to ω_0 . However, at finite temperatures $\Sigma_1(\omega)$ develops a resonance structure around ω_0 and two further crossings appear. At the middle crossing (the one with $\partial_\omega \text{Re}[\Sigma] > 0$) the self-energy has a large imaginary part, so that this does not correspond to a well-defined excitation; as a consequence, the spectrum contains now *two* quasiparticle solutions. The resonance at $\omega \sim \omega_0$ arises because the extended matrix $\tilde{\mathcal{T}}$ in (1) has a pole at $\tilde{\omega}_p = \epsilon_{\mathbf{p}} + \Sigma_0(\tilde{\omega}_p, \mathbf{p})$, which is very close to ω_0 for $T = 0$ and $\mathbf{p} \rightarrow 0$, since the number of excited bosons is negligible. For $T > 0$, the Bose distribution $f_{\mathbf{k}}$ is infrared divergent, which in combination with the pole of the $\tilde{\mathcal{T}}$ matrix means that the integrand in (3) for Σ_1 is very large for $\mathbf{k} \rightarrow 0$, changing sign around $\omega \sim \tilde{\omega} \approx \omega_0$. This results in the resonance structure shown in Fig. 5, a completely non-perturbative feature of the extended scheme. The energy splitting between ω_\uparrow and ω_\downarrow increases with temperature, since more particles are thermally excited out of the BEC leading to a more pronounced resonance structure. This explains the behaviour seen in Figs. 2-3.

The physical interpretation of the resonance feature of $\tilde{\mathcal{T}}$ is that the coupling between the impurity and the low-lying Bogoliubov modes gets strongly enhanced by the presence of the macroscopically occupied condensate modes for $\mathbf{k} \rightarrow 0$. The coupling to the BEC itself however is via the usual ladder scattering matrix \mathcal{T} . At finite temperatures $0 < T < T_c$, the impurity couples to both the BEC and a macroscopic amount of excited bosons, and the hybridization between these two terms leads to the emergence of two quasiparticles.

Increasing $k_n a_B$ has two main effects on the resonance structure of Σ . First, it becomes less pronounced, since the low-energy density-of-states of the BEC decreases due

to the stiffening of the Bogoliubov dispersion. Second, it moves to lower energies because of the increased effect of the coherence factors $u_{\mathbf{k}}, v_{\mathbf{k}}$. Indeed, in the weak coupling limit the resonance is approximately located at $n_0(\mathcal{T}_v - \mathcal{T}_B)$ [48] (these energies are plotted as vertical dashed lines in Fig. 5). It follows from these two effects that at low temperatures only *one* quasiparticle solution (the upper polaron) survives in the limit of weak impurity-bath coupling $|a| \lesssim a_B \ll 1/k_n$, and the energy of this solution approaches the first order result $n\mathcal{T}_v$, in agreement with perturbation theory [48].

An important question concerns whether three-body losses wash out the effects predicted in this paper. Three-body losses were investigated in the Aarhus and JILA experiments. Both groups found that they have surprisingly small effects, in the sense that the observed spectra could be explained theoretically without introducing three-body losses. Since our predicted temperature shifts and splittings have the same order of magnitude as the polaron energy at $T = 0$, we conclude that their observation is likely robust towards three-body losses.

Conclusions and outlook.— Using a diagrammatic resummation scheme designed to include scattering terms that are crucial at finite temperature, we showed that the Bose polaron has a highly non-trivial temperature dependence. For attractive interactions, the polaron splits into two quasiparticle states for $0 < T < T_c$. The energy of the lower polaron displays a minimum at T_c , whereas the energy of the upper one increases with T until its residue vanishes at T_c . These effects arise due to the coupling of the impurity to the Bogoliubov spectrum, whose population has an infrared divergence for finite temperature, and the enhancement of the coupling due to the presence of the condensate mode. Both the splitting of the polaron into two quasiparticles and the temperature dependence of their energies should be observable in experiments with ultracold gases, provided that specific care is taken to minimize the frequency and trap averaging of the spectral signal [19, 20].

Here we considered only negative energies. It would be interesting to investigate whether the discrepancy found in Ref. [19] between theory and experiment at positive energies could be due to finite temperature effects. A complete treatment of this subtle point requires a self-consistent calculation, which is beyond the scope of the present work, but a brief discussion of the matter is presented in the Supplemental Material [48].

Let us conclude by noting that the physical mechanism leading to the two main results of our paper, the strong temperature dependence and the quasiparticle splitting, is generic: both effects are caused by the condensed Bose gas breaking a continuous symmetry below T_c , so that a gapless mode appears, leading to a dramatic change in the low energy density of states to which the impurity couples. Our findings are therefore relevant to a wide class of systems consisting of an impurity immersed in a

medium breaking a continuous symmetry. This includes impurities in liquid Helium [3], normal and high- T_c superconductors [4], ultracold Fermi superfluids [18], and quantum magnets [49]. A similar splitting of a fermionic quasiparticle into two modes due to the coupling to a linear bosonic spectrum has indeed been predicted in hot quark-gluon plasmas, and in Yukawa and QED theories [40–43]. Due to its collective nature, the emergent quasiparticle was dubbed *plasmino* [50]. Our results therefore provide an avenue to study this interesting prediction in the controlled environment of a quantum gas.

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