

Quantum Impurities in Finite-Temperature Bose Gases: Detecting Vortex Proliferation across the BKT and BEC Transitions

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We propose a spectroscopic method to detect vortex proliferation in neutral superfluids that does not require spatially resolving individual vortices. Using stochastic classical-field methods, we theoretically show that a quantum impurity repulsively coupled to a weakly interacting Bose gas at finite temperature carries direct spectroscopic signatures of vortex proliferation. In two dimensions, we find that a low-energy (attractive) branch in the excitation spectrum becomes prominent when the temperature is tuned across the Berezinskii-Kosterlitz-Thouless (BKT) transition. We explain this red-shifted resonance as originating from the binding of the impurity to vortices, where the bosons density (and hence, the repulsive Hartree energy) is reduced. This mechanism could be exploited to spectroscopically estimate the BKT transition in excitonic insulators. In contrast, in three dimensions, the impurity spectra reflect the presence of vortex rings well below the condensation temperature, and herald the presence of a thermal gas above the Bose-Einstein transition. Importantly, we expect our results to have impact on the understanding of Bose-polaron formation at finite temperatures.

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Introduction—A mobile impurity immersed in a quantum background, commonly referred to as a *polaron*, provides a paradigmatic setting of quantum many-body physics [1–4]. An open problem in the field concerns the fate of polarons in a finite temperature Bose gas. Recent studies relied on perturbative calculations [5,6], time-dependent Hartree-Fock-Bogoliubov approach [7], diagrammatic ladder resummation [8], the functional renormalization group [9], and variational methods [10,11]. However, these techniques rely on a small temperature expansion. On the other hand, quantum Monte Carlo simulations can reach the condensation temperature [12], but do not provide access to spectral properties nor much physical insight. A generalized functional determinant approach has been used for the case of noninteracting bosons [13]. In cold atoms, Bose polarons were first observed in injection radio-frequency spectroscopy experiments [14,15], while ejection spectroscopy

unveiled the temperature-induced breakdown of quasiparticles in the critical regime of the mixture [16].

Polaron spectroscopy via optical injection of excitons is an emerging tool for transition-metal dichalcogenide (TMD) heterostructures [17,18]. The exciton acts as a sensor, and the quantum phase of the heterostructure reflects itself in the optical spectrum, in spite of the electronic dynamics occurring on length scales much smaller than the optical wavelength. Several experimental and theoretical works have demonstrated the sensitivity of polaron spectroscopy to the level of doping [17,18], the breaking of translational symmetry [19–24], the onset of insulating phases [25–28], and to the pairing of electrons and holes into excitonic insulators (EXI) [29,30], an exotic phase of matter recently observed in bilayers [31–33]. In particular, in bilayer EXIs, the optically injected *intralayer* exciton acts as impurity and interacts via short-range interactions with the *interlayer ground-state* excitons. While it has been predicted that at zero temperature the interlayer pairing can lead to exotic biexcitons and affects the optical spectrum [29], it is not clear whether superfluidity, a manifestation of quasi-long-range order, and the Berezinskii-Kosterlitz-Thouless (BKT) transition [34] can also be optically detected.

In this Letter, we study the injection spectra of an impurity repulsively coupled to a bath of weakly interacting

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bosons at finite temperatures, both in two (2D) and three (3D) spatial dimensions. We model the Bose gas via the stochastic projected Gross-Pitaevskii equation (SPGPE) [35,36], and consider the full Schrödinger equation for the impurity, which is injected at zero momentum. When the temperature is increased, a low-energy spectral line emerges when vortices and density holes appear in the bath. In 2D, our results suggest that polaron spectroscopy can be used to indirectly probe the BKT transition, which is associated with the proliferation of unbound vortices. In a similar spirit, it was recently demonstrated that indirect signatures of a topological insulator—a phase of matter characterized by a nonlocal topological invariant—can be obtained through polaron spectroscopy performed locally on its edge [37]. Also, it was recently predicted that, for *charged* superfluids (superconductors), local magnetometry provides a sensitive probe of the phase gradient of the quasicondensate, and can provide evidence for the BKT transition [38]. In 3D, instead, we find that vortex rings proliferate well below the critical temperature of the Bose-Einstein condensate (BEC), above which the repulsive branch disappears.

Detecting vortices through classical microparticles has been exploited in the context of helium [39]. Therefore, on the one hand, our approach is a generalization of this method to the realm of quantum impurities. On the other hand, the crucial difference is that here we do not require the capability of spatially resolving the impurity, but its wavelike interaction with the vortices results in characteristic spectral lines. Our proposed scheme can be directly implemented in cold-atom setups and provides a route to indirectly probe the BKT transition in the EXIs hosted in 2D materials, where the relevant electronic length scales are well below the optical diffraction limit. The Letter is structured as follows: we first define the model and impurity spectra, review the SPGPE, and then discuss our results in 2D and 3D. Finally, implications for the EXI and future prospects are discussed.

Model and methods—Considering for simplicity contact interactions [40], an impurity in a weakly interacting Bose gas is described (in units $\hbar = 1$) by the Hamiltonian

$$\hat{H} = \int d\mathbf{x} \left\{ \hat{\psi}^\dagger \left(-\frac{1}{2m} \nabla^2 - \mu \right) \hat{\psi} - \frac{1}{2M} \hat{\Psi}^\dagger \nabla^2 \hat{\Psi} + \frac{g_{\text{BB}}}{2} \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} + g_{\text{BI}} \hat{\psi}^\dagger \hat{\psi} \hat{\Psi}^\dagger \hat{\Psi} \right\}, \quad (1)$$

where $\hat{\psi}^\dagger(\mathbf{x})$ creates a boson at position $\mathbf{x}$ in a d -dimensional box of volume V , and $\hat{\Psi}^\dagger(\mathbf{x})$ is the impurity creation operator (the quantum statistics of the impurity is irrelevant in this work). The corresponding masses are m and M , μ is the chemical potential of the Bose gas, and g_{BB} and g_{BI} are the strength of the repulsive boson-boson and boson-impurity interactions, respectively.

For the injection spectra of the impurity within the Bose gas at finite temperature, the main observable is provided by the overlap function

$$S(t) = \text{Tr}[\hat{\Psi}_{\mathbf{q}=0}(t) \hat{\Psi}_{\mathbf{q}=0}^\dagger(0) \hat{\rho}(0)], \quad (2)$$

where $\hat{\Psi}_{\mathbf{q}=0}^\dagger(t)$ is the creation operator of the impurity at zero momentum and time t , and $\hat{\rho}(0)$ represents the density matrix of the system just before the injection of the impurity, comprising the thermal equilibrium density matrix of the bath times the impurity vacuum. The frequency-resolved spectrum is $A(\omega) = -2 \text{Im} S(\omega)$, obtained by Fourier transforming $S(t)$. The choice of this observable is motivated by TMD experiments, where the exciton is optically injected with negligible momentum, with respect to the electronic scales. In an ultracold atomic gas, one would initially prepare the impurity separately from the bath, and then quench the interactions.

For ultracold gases, classical-field methods, such as the GPE equation and its generalizations, provide an excellent description of the weakly interacting Bose gas, both at zero and finite temperature, at equilibrium or in the dynamics [42–45]. In particular, the SPGPE has been recently used to study the vortex formation dynamics across the BEC [46] and BKT [43] phase transitions.

Building on this framework, we assume that the bath consists of $N \gg 1$ bosonic atoms described at the mean-field level, while we treat the impurity atom using its full Schrödinger equation. Let us denote by ψ the semiclassical field that represents the Bose gas, and by Ψ the quantum wave function of the impurity. In the SPGPE scheme, the equations of motion read [35,36,47–49]

$$i\partial_t \psi = \mathcal{P}(1 - i\gamma) \left\{ -\frac{1}{2m} \nabla^2 + g_{\text{BB}} |\psi|^2 - \mu \right\} \psi + \eta, \quad (3)$$

$$i\partial_t \Psi = \left\{ -\frac{1}{2M} \nabla^2 + g_{\text{BI}} n_{\text{B}} \right\} \Psi. \quad (4)$$

The Bose gas exchanges energy and particles with a thermal reservoir at temperature T and chemical potential μ , and encompasses contributions from all highly occupied single-particle modes of the system, up to an energy cutoff. The projection operator, implemented in momentum space by $\mathcal{P} = \theta[\epsilon_{\text{cut}} - (\mathbf{k}^2/2m)]$, prevents population transfer beyond the coherent region, i.e., the single-particle modes below the cutoff energy $\epsilon_{\text{cut}} = \mu + T \log 2$ (in units where the Boltzmann constant is one). This cutoff sets an order ~ 1 mean occupation number, assuming a noninteracting Bose-Einstein distribution [48]. The white noise η , added and projected in the coherent region, has a variance dictated by the fluctuation-dissipation theorem, $\langle \eta^*(\mathbf{x}, t) \eta(\mathbf{x}', t') \rangle = 2\gamma T \delta(t - t') \delta(\mathbf{x} - \mathbf{x}')$. The effective dissipation rate γ specifies the strength of the coupling between the system and the thermal bath.

The Bose gas density is $n_B(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2 + n_{\text{inc}}$, with $n_{\text{inc}} = \int [d\mathbf{k}/(2\pi)^d] \{ [\theta(|\mathbf{k}| - k_{\text{cut}})] / [e^{k^2/2mT} - 1] \}$, the incoherent part, which keeps into account the occupation of the bosonic modes above the cutoff $\varepsilon_{\text{cut}} = k_{\text{cut}}^2/(2m)$. In 2D, this translates into $n_{\text{inc}} = (m/2\pi)T \log 2$, and to $n_{\text{inc}} \simeq 0.059(mT)^{3/2}$ in 3D.

In principle, a term $g_{\text{BI}}|\Psi|^2\psi$ should appear in Eq. (3). However, the bosonic field intensity $|\psi|^2$ is of order N/V , while the impurity wave function is normalized, so that $|\Psi|^2$ is of order $1/V$ and goes to zero in the thermodynamic limit. In other words, when performing linear polaron spectroscopy on a large sample, the recoil of the quasi-condensate due to the impurity can be neglected, since a single delocalized impurity cannot impact the many-body (quasi)condensate. This assumption breaks down for extremely strong impurity-boson repulsion $g_{\text{BI}} \sim Ng_{\text{BB}}$, where self-localization phenomena may emerge [50]. Also, the attractive case $g_{\text{BI}} < 0$ is beyond the reach of our method, since a bound state of the impurity with a single boson would play a major role [51]. The GPE approach has been recently applied to model the strong deformation of the bosonic bath by the impurity at zero temperature [59–61].

In our framework, the impurity is described by a Schrödinger equation with a stochastic time-dependent external potential. Then, the overlap of Eq. (2) reduces to $S(t) = \langle\langle \Psi_{\mathbf{q}=0}(t) \rangle\rangle$, where the double brackets $\langle\langle \dots \rangle\rangle$ denote stochastic averages. Here, $\Psi(\mathbf{x}, t)$ denotes the impurity wave function at time t , obtained from the Schrödinger equation (4) with uniform initial condition $\Psi(\mathbf{x}, 0) = (1/\sqrt{V})$. Numerically, for each stochastic realization, the bath is equilibrated by evolving a uniform initial state ψ via the SPGPE for a duration t_{eq} until $t = 0$, at which time the impurity is initialized at momentum $\mathbf{q} = 0$ and its evolution recorded. This procedure is averaged over M_{stat} stochastic realizations. The chemical potential is adjusted with temperature to fix the average bosonic density $\langle\langle n_B \rangle\rangle = n_0$, with n_0 independent of T .

Numerical results in 2D—The Mermin-Wagner theorem prevents the existence of a local order parameter for the 2D Bose gas at any finite temperature. Nonetheless, at low temperature, the field-field correlation function decays only algebraically $\langle\langle \psi^*(\mathbf{x})\psi(\mathbf{x}') \rangle\rangle \propto |\mathbf{x} - \mathbf{x}'|^{-\alpha}$, with a critical exponent $\alpha(T)$, and a fraction ρ_S of the bosons display superfluid behavior. For a weakly interacting gas, the BKT transition occurs at the temperature [62]

$$T_{\text{BKT}}^\infty = \frac{2\pi n_0}{m \log\left(\frac{C}{mg_{\text{BB}}}\right)}, \quad (5)$$

with $C \simeq 380$; ρ_S drops to zero at T_{BKT}^∞ and the critical exponent is $\alpha(T_{\text{BKT}}^\infty) = 1/4$. The transition corresponds to the unbinding of vortex-antivortex pairs and is of topological nature. On the other hand, the quasicondensate

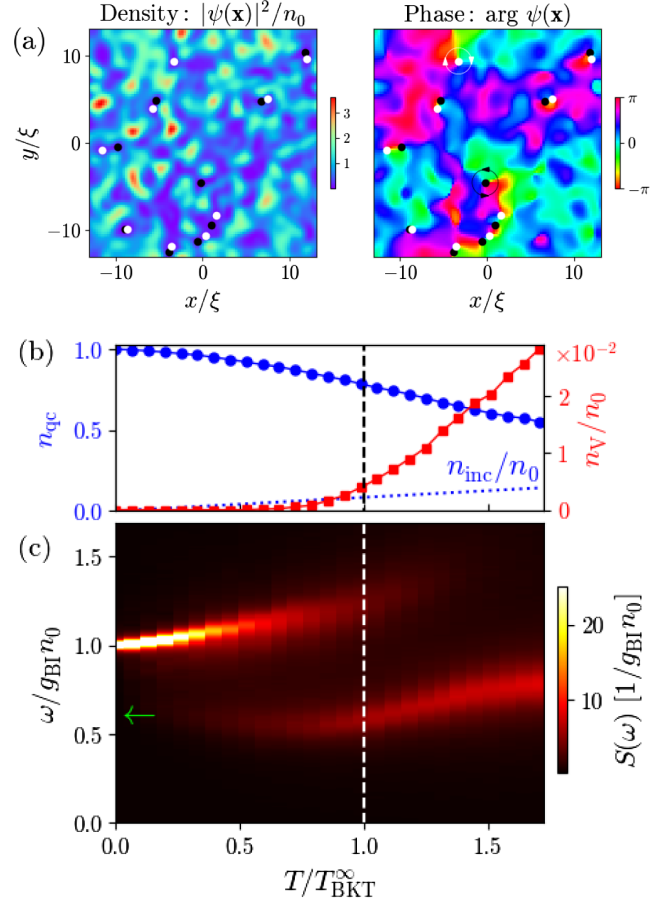


FIG. 1. BKT phase diagrams and 2D injection spectra. (a) For the 2D Bose gas without impurity, we report a typical snapshot of the density (left) and of the phase (right) of the quasicondensate at $T \simeq 1.05T_{\text{BKT}}$. The black and white dots denote vortices and antivortices, respectively. Apart from a few bound vortex-antivortex pairs, one can spot two unbound vortices, with the phase performing a full $\pm 2\pi$ winding over a large distance (highlighted by the circulation of the arrows). The healing length $\xi = (2mg_{\text{BB}}n_0)^{-1/2}$ provides the natural length scale for the variations of ψ . (b) We plot the quasicondensate fraction n_{qc} (blue circles, left axis), the incoherent density n_{inc} (blue dots), and the density of vortices (red squares, right axis) as a function of temperature. Error bars are smaller than the marker size. (c) The injection spectrum $S(\omega)$ of the impurity is plotted as a function of T , in the equal mass $M = m$ case. The green arrow indicates the binding energy of the impurity in an isolated vortex at $T = 0$. The attractive branch $S(\omega)$ displays a minimum close to the BKT transition, where vortices starts to proliferate. The colorcode is saturated and the lines slightly broadened, since at vanishing temperature $S(\omega)$ becomes a δ peak.

fraction $n_{\text{qc}} = \sqrt{2\langle\langle |\psi|^2 \rangle\rangle^2 - \langle\langle |\psi|^4 \rangle\rangle} / \langle\langle |\psi|^2 \rangle\rangle$ is smooth at threshold, since it is a local quantity. (A previous polaron model assumed a jump of n_{qc} at T_{BKT}^∞ [63].)

This BKT physics is perfectly recovered at the equilibration step of our numerical simulations, as illustrated in Fig. 1. In Fig. 1(a) we report a typical snapshot of the

density and phase of the bosonic mean-field ψ , revealing strong density fluctuations, as well as many vortex-antivortex pairs, indicated by the black and white points. Above the BKT transition, a fraction of the pairs unbind (one out of nine in this snapshot). In Fig. 1(b), we study how statistical properties vary with temperature. The blue circles correspond to the quasicondensate fraction, n_{qc} which decreases smoothly with T . We point out that the incoherent fraction n_{inc}/n_0 (blue dotted line) is around 8% at the critical temperature, for our system parameters, and we verified that all our conclusions are insensitive to the precise value of ϵ_{cut} [52]. The density of vortices n_V , evaluated from the vortex circulation around closed paths on the numerical grid is shown in red squares (right axis). As expected [43], a few (bound) vortices are found at temperatures slightly below T_{BKT}^∞ , and n_V increases steadily with temperature for $T > T_{BKT}^\infty$. Thus, one can say that vortex proliferation is a precursor of the BKT transition. We show in Supplemental Material [52] that the values of n_{qc} and n_V as well as the impurity spectrum are well converged for our box size, and can thus be interpreted as *local* observables. There, we also report the critical exponent $\alpha(T/T_{BKT}^\infty)$, which accounts for quasi-long-range order. As it is well known [62], the *nonlocality* of this quantity results in logarithmic corrections with the system size; nonetheless, for the largest system sizes, the critical value $\alpha = 1/4$ is achieved for temperatures consistent with $T \sim T_{BKT}^\infty$. The fact that the impurity spectra discussed below are well converged with the system size confirms the locality of the impurity probe, and its insensitiveness to quasi-long-range order.

In the equal mass case $M = m$, and setting $g_{BI} = 2g_{BB}$, the impurity spectral function $S(\omega)$ is shown in Fig. 1(c), as a function of temperature. At low temperatures, the Bose gas can be approximated as a uniform background of density n_0 , and the impurity spectrum behaves as a deltalike peak centered at $\omega = g_{BI}n_0$. At higher temperatures, density fluctuations become important; in particular, vortices are nucleated already slightly below T_{BKT}^∞ , where the field develops points of zero density. Conversely, it seems that not all density holes correspond to vortices, as visible from the strong density fluctuations in typical snapshots of the Bose gas [see Fig. 1(a)]. Thus, the impurity-boson interaction being repulsive, the impurity can bind to regions of low density. Indeed, the green arrow in Fig. 1(c) indicates the bound state energy of the impurity within a single vortex, assuming a $T = 0$ static gas. This binding results in the phenomenology observed in Fig. 1(c) at intermediate temperatures, where two spectral lines are reminiscent of the usual repulsive and attractive polaron branches. The attractive branch appears to have a minimum around the proliferation threshold at $T \sim 0.85T_{BKT}^\infty$, and displays a natural broadening. The blueshift of the attractive branch above T_{BKT} is in part due to the increase of the incoherent fraction, which provides a uniform blueshift. A

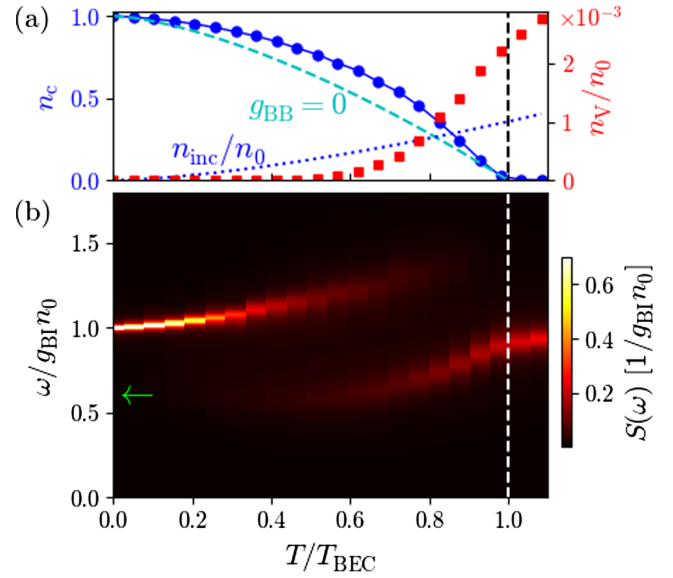


FIG. 2. BEC phase diagram and injection spectra for the 3D case. For the 3D Bose gas without impurity, we plot as a function of temperature the condensate fraction n_c (blue circles, left axis), the incoherent density n_{inc} (blue dots), and the density of (projected) vortex ring points (red squares, right axis). (b) The injection spectrum $S(\omega)$ of the impurity is plotted as a function of T , in the equal mass $M = m$ case. The green arrow indicates the binding energy of the impurity in an isolated vortex at $T = 0$. The attractive branch $S(\omega)$ displays a minimum close to the threshold for vortex ring nucleation, while above the condensation temperature T_{BEC} one observes a single Lorentzian peak. The color code is slightly saturated.

quantum Monte Carlo study of repulsive impurities [12] identified a similar dependence of the ground-state energy with T . A nontrivial, multibranch behavior is observed when the mass ratio is varied, as discussed in the End Matter.

Numerical results in 3D—It is equally interesting to consider the impurity injection into a 3D Bose gas. The physics of the Bose gas in the absence of the impurity and for increasing temperature is illustrated in Fig. 2(a). First, the condensed fraction $n_c = \langle |\psi_{\mathbf{k}=0}|^2 \rangle / n_0$ (blue circles, left axis) is lower bounded by the noninteracting, textbook result $n_c(g_{BB} = 0) = 1 - (T/T_{BEC})^{3/2}$, indicated by the cyan dashed line, and vanishes close to the BEC condensation temperature $T_{BEC} \simeq 3.3125n^{2/3}/m$ [41]. The blue dotted line denotes the incoherent fraction. A very interesting aspect of the 3D Bose gas at finite temperature, which to our knowledge has not been investigated before, is the presence of vortex rings well below T_{BEC} . These rings are analogous to paired vortices, and do not spoil the long-range order. We detect the rings by the application of the 2D vortex detection algorithm, by slicing the 3D space along each of the three directions separately. The density of vortical points is plotted as red squares in Fig. 2(a) (right axis). A snapshot of the vortex rings is reported in Fig. S12 of Supplementary Material [52].

The impurity injection spectra, calculated for parameters suitable to Rubidium experiments and with $M = m$, show similar features as the 2D ones, with the presence of the attractive line correlated to the nucleation of vortex rings; cf. Fig. 2(b). At the BEC transition, however, the vanishing of the condensate fraction entails that the fluid behaves like a uniform thermal gas. As a consequence, the spectrum features a single peak around $\omega \sim gn_0$.

Conclusions and discussion—In summary, we computed the injection spectra of an impurity in a weakly interacting Bose gas at finite temperature, using stochastic classical-field methods and for repulsive impurity-boson interactions. The binding of the impurity to vortices and density holes makes the spectra sensitive to vortex proliferation, a precursor of the BKT transition in 2D; in 3D, instead, we found that vortex nucleation and condensation occur at substantially different temperatures. In our numerics, we took parameters from ultracold experiments with Rubidium.

Our work opens several intriguing directions. First, it suggests that it may be possible to obtain indirect signatures of the nonlocal BKT transition via a local probe, which may enable the detection of superfluidity in TMD EXI experiments. While a microscopic calculation would be extremely complex and is beyond the scope of this work, we will provide numerical estimates for the visibility of a double peak structure in the repulsive polaron branch of the intralayer exciton spectrum. The Mott transition in TMD bilayers is estimated to occur at an interlayer exciton density of $1 - 2 \times 10^{12} \text{ cm}^{-2}$ [31,64]. We assume that at $5 \times 10^{11} \text{ cm}^{-2}$ we can neglect fermionic effects and deal with a (strongly interacting) Bose gas, eluding a GPE description. Quantum fluctuations due to repulsive dipolar interactions can lead, even at zero temperature, to a filling of the vortex core by a noncondensed fraction. We assume that this effect leads to a 50% reduction of the vortex density depletion (in superfluid helium it is estimated that the reduction is by 40% [65]). For the strength of the intralayer-interlayer exciton interactions, since the biexciton binding energy in vacuum is comparable with the trion [29], it is reasonable to take the repulsive branch blueshift at zero temperature as the one of the monolayer at the same density, thus of the order of 5 meV [21]. The mass ratio between the interlayer and intralayer exciton is approximately 1, as in Fig. 1, and we can expect that at the BKT transition (expected at temperatures in the range of 10–50 K), the splitting of the repulsive branch, which is of the order of half the blueshift in Fig. 1, is halved to one quarter due to the quantum filling of the vortex core. This means that the repulsive exciton line should display a splitting of 1–2 meV, which is comparable with its linewidth in samples optimized for optical spectroscopy. A more detailed modeling, including the fermionic and dipolar nature of the exciton fluids [66,67], will be pursued in the future. Driven-dissipative polariton fluids, where the onset

of BKT physics can be imaged on the micrometer scale [68,69], also deserve attention.

Moreover, our results bear strong implications for the more conventional Bose polaron setup, i.e., with *attractive* impurity-boson interactions, for which no reliable spectral predictions are available beyond small temperatures. We expect the repulsive branch to be effectively described by the present formalism, and to feature a splitting at finite temperatures. This claim (as well as modifications in the genuinely attractive branch) should be investigated in future work. A promising strategy for future research would be to apply the finite temperature Lee-Low-Pines transformation [11] and adopt the GPE in this frame [59].

Finally, it is worth exploring the recoil of the bosons and the effect of a finite density of impurities on the BKT transition, as well as the case of interacting impurities.

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Data availability—The data that support the findings of this article are openly available at [70].

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End Matter

In the main text we focused on the equal mass case, which is most relevant for both cold atoms and TMD experiments. However, a very rich behavior is found when the boson-impurity mass ratio is varied, to which we devote some analysis in this end matter. For the light impurity of mass $M = 0.5m$ reported in Fig. 3(a), a single line dominates the spectrum at all temperatures, which is broadest at intermediate temperatures. As shown in Sec. S9 of [52], a similar spectrum is obtained when freezing the bath dynamics, suggesting that the light impurity is fast enough to cancel out the time dependence of the bath and effectively experience a static bath density. We then speculate that the presence of a unique line is related to the fact that, in a closed system, the ground state wave function can always be chosen real and positive, entailing a sizable zero momentum component; as a consequence, low lying energy states would carry most of the oscillator strength.

On the contrary, for the heavier impurity with $M = 2m$ shown in Fig. 3(b), one recovers a repulsive line, as in Fig. 1(b), but the attractive features are quite different. First of all, two attractive lines are visible (see the inset), and we relate this to the fact that for this mass ratio the single vortex admits now two s -wave impurity bound states, whose energies are studied in panel (c). Furthermore, the attractive lines are very weak and broad (notice that the colorscale has been saturated to make these lines more visible).

In Ref. [52] we also calculated the injection spectra for attractive boson-impurity interactions. In this case, only one line is present, broadening with increasing temperatures. The absence of a lower lying peak is probably due to the fact that bumps of high density have a very fast dynamics, and do not support proper bound states, like vortices do in the repulsive case.

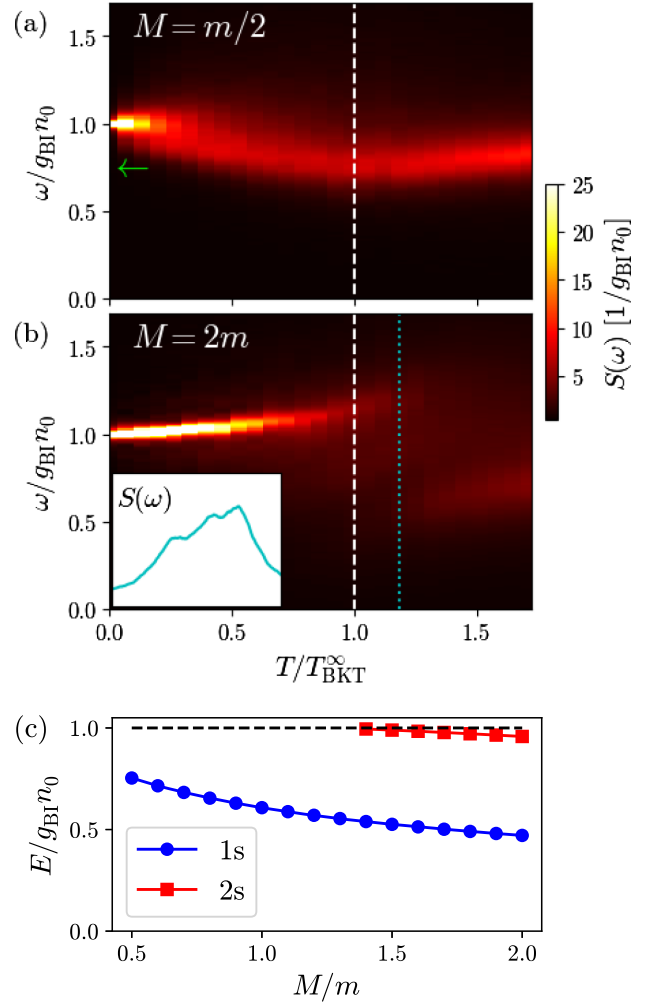


FIG. 3. Injection spectra for impurities of varying masses. Injection spectra as a function of the temperature, analogous to Fig. 1(b), are reported for a lighter $M = m/2$ and a heavier $M = 2m$ impurity, in panels (a) and (b), respectively. In the inset of panel (b), we show that a three peak structure is present for a spectral slice at $T \simeq 1.2 T_{\text{BKT}}^{\infty}$ (corresponding to the vertical dotted line in the main figure). In panel (c), the binding energy of the impurity in an ideal vortex is studied as a function of the impurity mass. A $2s$ bound state is supported for heavy enough impurities (red squares).