Phase transitions in the boson-fermion resonance model in one dimension

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We study one-dimensional fermions with photoassociation or with a narrow Fano-Feshbach resonance described by the boson-fermion resonance model. Using the bosonization technique, we derive a low-energy Hamiltonian of the system. We show that at low energy, the order parameters for the Bose condensation and fermion superfluidity become identical, while a spin gap and a gap against the formation of phase slips are formed. As a result of these gaps, charge density wave correlations decay exponentially in contrast with the phases where only bosons or only fermions are present. We find a Luther-Emery point where the phase slips and the spin excitations can be described in terms of pseudofermions. This allows us to provide closed form expressions of the density-density correlations and the spectral functions. The spectral functions of the fermions are gapped, whereas the spectral functions of the bosons remain gapless. The application of a magnetic field results in a loss of coherence between the bosons and the fermion and the disappearance of the gap. Changing the detuning has no effect on the gap until either the fermion or the boson density is reduced to zero. Finally, we discuss the formation of a Mott insulating state in a periodic potential. The relevance of our results for experiments with ultracold atomic gases subject to one-dimensional confinement is also discussed.

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I. INTRODUCTION

Since the discovery of Bose-Einstein condensation (BEC) of atoms in optical traps, the field of ultracold atoms has experienced tremendous developments in recent years [1]. A first important step has been the use of Fano-Feshbach resonances [2,3] to tune the strength of atom-atom interaction [4–6]. Fano-Feshbach resonances take place when the energy difference between the molecular state in the closed channel and the threshold of the two-atom continuum in the open channel, known as the detuning ν, is zero [7]. Near a Fano-Feshbach resonance, the atom-atom scattering length possesses a singularity. For $\nu>0$, atoms are stable, but the existence of the virtual molecular state results in an effective attraction. For $\nu<0$, the molecules are formed and possess a weakly repulsive interaction. Since the value of ν can be controlled by an applied magnetic field, this allows one to tune the sign and strength of the atomic and molecular interactions [8–11]. In particular, the use of Fano-Feshbach resonances has allowed the observation of pairs of fermionic [12–15] or bosonic [16–19] atoms binding together to form bosonic molecules. At sufficiently low temperature, for $\nu<0$, these molecules can form a Bose-Einstein condensate. In the case of a fermionic system, for $\nu>0$, due to attractive interactions a BCS superfluid is expected. Since the BEC and the BCS state break the same U(1) symmetry, a smooth crossover between the two states is expected as ν is tuned through the resonance. Indeed, the BEC of molecules [12,20,21] and the crossover to a strongly degenerate Fermi gas [22–25] have been observed as a gas of cold fermionic atoms is swept through the Fano-Feshbach resonance. Measurement of the radio-frequency excitation spectra [26] and of the specific heat [27] as well as observation of vortices in a rotating system [28] on the $\nu>0$ side revealed the presence of a superfluid BCS gap, thus proving the existence of a BEC-BCS crossover. Such a crossover is naturally described by the boson-fermion model [29–36], first introduced in the 1950s in the context of the theory of superconductivity [37,38] and later reinvestigated in the 1980s in the context of polaronic [39] and high-T_c superconductivity theory [40–42]. A second important parallel development has been the possibility to form quasi-one-dimensional condensates using anisotropic traps [43–46], two-dimensional optical lattices [47–52], or atoms on chips [53]. In one-dimensional systems interactions are known to lead to a rich physics [54]. In particular, strongly correlated states of fermions, where individual particles are replaced by collective spin or density excitations, are theoretically expected [54–56]. When the interactions between the fermions are repulsive, both the spin and density fluctuations are gapless with linear dispersion and this state is known as the Luttinger liquid [54,57,58]. For attractive interactions between the fermions, the spin degrees of freedom develop a gap, yielding a state known as the Luther-Emery liquid [54,59]. Similarly, bosons are expected to be found in a Luttinger liquid state, with individual particles being replaced by collective density excitations [54,55,60,61]. Moreover, strong repulsion can lead to the fermionization of interacting bosons, i.e., the density matrix becomes identical to that of a noninteracting spinless fermion system, the so-called Tonks-Girardeau (TG) regime [62,63]. Experiments in elongated traps have provided evi-

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dence for one-dimensional (1D) fluctuations [44–46]. However, in these systems, the bosons remain weakly interacting. With two-dimensional optical lattices, it is possible to explore a regime with stronger repulsion. In particular, it was possible to observe the TG regime with ^{87}Rb atoms [49] by increasing the transverse confinement. The TG regime can also be reached by applying a 1D periodic potential along the tubes to increase the effective mass of the bosons [50]. Using a stronger 1D potential, it is possible to drive a one-dimensional Mott transition between the superfluid state and an insulating state [51]. Another characteristic of atoms in a one-dimensional trap is that transverse confinement can give rise to a type of Fano-Feshbach resonance as a function of the trapping frequency called the confinement induced resonance (CIR) [64–66]. Recently, experiments have been performed on ^{40}K fermionic atoms in a one-dimensional trap forming bound states either as a result of Fano-Feshbach resonances or of CIR [67]. Both types of bound states have been observed and the results can be described using the Boson-Fermion model [68]. This prompts the question of whether a one-dimensional analogue of the BEC-BCS crossover could be observed in such a system. It is well known that in one dimension, no long range BEC or BCS order can exist [69–71]. However, quasi-long range superfluid order is still possible. For fermions with attractive interactions, it was shown using the exactly solved Gaudin-Yang model [72,73] that for weakly attractive interactions, a Luther-Emery state with gapless density excitations and gapful spin excitations was formed, whereas for strongly attractive interactions the system would crossover to a Luttinger liquid of bosons [74,75]. The boson-fermion model was also considered in the case of a broad Fano-Feshbach resonance [76]. In that case only bosons or fermions are present (depending on which side of the resonance the system is) and the results are analogous to those obtained with the Gaudin-Yang model. In fact, in the three-dimensional case, it is possible to derive a mapping of the boson-fermion model with a broad resonance to a model with only fermions and a two-body interaction [77]. In the narrow resonance case, such a mapping is valid only very close to the resonance. It was therefore interesting to investigate what happens in one dimension in the case of a narrow resonance. Indeed, in the latter case, it has been shown previously [78,79] that a richer phase diagram could emerge with a phase coherence between a fluid of atoms and a fluid of molecules at weak repulsion and a decoupling transition for stronger repulsion. Analogous effects have been discussed in the context of bosonic atoms with a Fano-Feshbach resonance in Ref. [80]. Due to the concrete possibility of forming 1D Fermi and Bose gas with optical lattices [52,61] some of the theoretical predictions in the narrow resonance case may become testable experimentally in the future. Experimental signature of the phase coherence between the two fluids include density response and momentum distribution function. In the present paper, we investigate in more detail the phase in which the atomic and the molecular fluid coexist. In particular, we study the equilibrium between the atomic and the molecular fluid as the detuning is varied. Also, we investigate the effect of placing the system in a periodic potential and show that the phase coherence between the atomic and molecular fluid hinders the formation of the Mott state in systems at commensurate filling. Such conclusion is in agreement with a study in higher dimension [81].

The plan of the paper is the following. In Sec. II we introduce the boson-fermion Hamiltonian both in the lattice representation and in the continuum. We discuss its thermodynamics in the limit of an infinitesimal boson-fermion conversion term and show under which conditions atoms and molecules can coexist. In Sec. III we derive the bosonized expression for the boson-fermion Hamiltonian valid in the region where atoms and molecules coexist. This Hamiltonian is valid for a system in an optical lattice provided it is at an incommensurate filling (i.e., with a number of atoms per site which is not integer). We show that for not too strong repulsion in the system, a phase where the atomic and the molecular superfluid become coherent can be obtained. This phase possesses a spin gap. We show that in this phase the order parameter for the BEC and the BCS superfluidity order parameter are identical, while charge density wave correlations present an exponential decay. We discuss the phase transitions induced by the detuning, the magnetic field, and the repulsion. We also exhibit a solvable point where some correlation functions can be obtained exactly. In Sec. IV, we consider the case where the number of atoms per site in the optical lattice is integer. We show that a phase transition to a Mott insulating state can be obtained in that case. However, there is no density wave order in this Mott state. Finally, in Sec. V, we discuss the applicability of our results to experiments.

II. HAMILTONIANS AND THERMODYNAMICS

A. Hamiltonians

We consider a system of 1D fermionic atoms with a Fano-Feshbach resonance [4–6,30]. This 1D system can be obtained by trapping the fermions in a two-dimensional or a three-dimensional optical lattice. In the first case, the fermions are trapped into 1D tubes, in the second case, a periodic potential is superimposed along the direction of the tubes. In the case in which the fermions are injected in a uniform potential, the Hamiltonian of the system reads

$$H = -\int dx \sum_{\sigma} \psi_{\sigma}^{\dagger} \frac{\nabla^2}{2m_F} \psi_{\sigma} + \int dx \psi_b^{\dagger} \left(-\frac{\nabla^2}{2m_B} + \nu \right) \psi_b + \lambda \int dx (\psi_b^{\dagger} \psi_{\uparrow} \psi_{\downarrow} + \psi_{\downarrow}^{\dagger} \psi_{\uparrow}^{\dagger} \psi_b) + \frac{1}{2} \int dx dx' \Bigg[V_{BB}(x-x') \times \rho_b(x) \rho_b(x') + V_{FF}(x-x') \times \sum_{\sigma,\sigma'} \rho_{\sigma}(x) \rho_{\sigma'}(x') + 2V_{BF}(x-x') \sum_{\sigma} \rho_{\sigma}(x) \rho_b(x') \Bigg], \quad (1)$$

where ψ_b annihilates a molecule, ψ_{σ} a fermion of spin σ, m_F is the mass of the isolated fermionic atom, $m_B = 2m_F$ the mass of the molecule, V_{BB}, V_{BF}, V_{FF} are (respectively) the molecule-molecule, atom-molecule and atom-atom interactions. Since these interactions are short ranged, it is convenient to assume that they are of the form $V_{\alpha\beta}(x) = g_{\alpha\beta}\delta(x)$. The term ν is the detuning. Finally, the term λ allows the

transformation of a pair of fermions into a Fano-Feshbach molecule and the reverse process. This term can be viewed as a Josephson coupling [82] between the order parameter of the BEC of the molecules, and the order parameter for the superfluidity of the fermions. As a result of the presence of this term, pairs of atoms are converted into molecules and vice-versa, as in a chemical reaction [37]. As a result of this, only the total number of atoms (paired and unpaired), $\mathcal{N}=2N_b+N_f$ (where N_b is the number of molecules and N_f is the number of unpaired atoms) is a conserved quantity.

In the case where atoms are injected in a periodic potential, $V(x)=V_0\sin^2(\pi x/d)$ it is convenient to introduce the Wannier orbitals [83] of this potential. In the single band approximation the Hamiltonian reads [84–87]

$$H=-t\sum_j (f^\dagger_{j+1,\sigma}f_{j,\sigma}+f^\dagger_{j,\sigma}f_{j+1,\sigma})+U\sum_j n_{f,j,\uparrow}n_{f,j,\downarrow}$$
$$-t'\sum_j (b^\dagger_{j+1}b_j+b^\dagger_j b_{j+1})+U'\sum_j (n_{b,j})^2+\nu\sum_j b^\dagger_j b_j$$
$$+\bar{\lambda}\sum_j (b^\dagger_j f_{j,\uparrow}f_{j,\downarrow}+f^\dagger_{j,\uparrow}f^\dagger_{j,\downarrow}b_j)+V_{BF}\sum_j n_{b,j}(n_{f,j,\uparrow}+n_{f,j,\downarrow}), \quad (2)$$

where $f_{j,\sigma}$ annihilates a fermion of spin σ on site j, $n_{f,j,\sigma}=f^\dagger_{j,\sigma}f_{j,\sigma}$, $b^\dagger_j$ creates a Fano-Feshbach molecule (boson) on the site j, and $n_{b,j}=b^\dagger_j b_j$. The hopping integrals of the fermions and bosons are, respectively, t and t'. The quantity ν is the detuning. The parameters U, U', and V_{BF} measure (respectively) the fermion-fermion, boson-boson, and fermion-boson repulsion. The case of hard core bosons corresponds to $U'\to\infty$. The conversion of atoms into molecules is measured by the term $\bar{\lambda}$. Again, only the sum $\mathcal{N}=2N_b+N_f$ is conserved. We note that within the single band approximation, there should exist a hard core repulsion between the bosons.

B. Thermodynamics of the boson-fermion model in the limit of $\lambda\to 0$

In this section, we wish to study the behavior of the density of unpaired atoms ρ_f and of the density of atoms paired in molecules ρ_b as a function of the total density of atoms (pair and unpaired) $\rho_{\text{tot.}}$ in the limit of $\lambda\to 0_+$. In such a limit, the fermion-boson conversion does not affect the spectrum of the system compared to the case without fermion-boson conversion. However, it is imposing that only the total number of atoms $\mathcal{N}=2N_B+N_F$ is conserved. Therefore, in this limit there is a single chemical potential $\mu=\mu_F$ and the chemical potential of the molecules is $\mu_B=2\mu$. If we further assume that $V_{BF}=0$, the Hamiltonian of the system can be decomposed as $H=H_f+H_b$, where H_f is the Hamiltonian of the unpaired atoms subsystem and H_b is the Hamiltonian of the molecules subsystem, and the partition function factorizes as $Z[\mu]=Z_f[\mu_F=\mu]Z_b[\mu_B=2\mu]$, where $Z_\nu[\mu_\nu]=\text{Tr}[e^{-\beta[H_\nu-\mu_\nu N_\nu]}]$ for $\nu=F,B$. Thus, in the limit λ, $V_{BF}\to 0$, we obtain the following expression of the number of unpaired atoms N_F and the number of atoms paired in molecules N_B:

$$N_F=\frac{1}{\beta Z_F}\left(\frac{\partial Z_F}{\partial\mu_F}\right)_{\mu_F=\mu}, \quad (3)$$

$$N_B=\frac{1}{\beta Z_b}\left(\frac{\partial Z_b}{\partial\mu_B}\right)_{\mu_B=2\mu}. \quad (4)$$

Equations (3) and (4) can be used to study the coexistence of bosons and fermions as the detuning ν is varied. Two simple cases will be analyzed to illustrate this problem of coexistence. First, we will consider bosonic molecules with hard core repulsion and noninteracting fermionic atoms. In such a case, the thermodynamics of the gas of molecules is reduced to that of a system of spinless fermions by the Jordan-Wigner transformation [62,63,88], and the expression of the densities of unpaired atoms and molecules can be obtained in closed form. In this simple case, it is straightforward to show that for sufficiently negative detuning all atoms are paired into molecules, and for sufficiently positive detuning all the atoms remain unpaired. The case of intermediate detuning is more interesting as coexistence of unpaired atoms with atoms paired into molecules becomes possible. The physical origin of this coexistence is of course the molecule-molecule repulsion that makes the chemical potential of the gas of molecules increase with the density so that in a sufficiently dense gas of molecules, it becomes energetically favorable to create unpaired atoms. To show that the above-noted result is not an artifact of having a hard core repulsion, we have also considered a slightly more realistic case of molecules with contact repulsion and noninteracting atoms. Although in that case we can no longer obtain closed form expressions of the density of molecules, we can still calculate numerically the density of molecules using the Lieb-Liniger solution [89]. We will see that having a finite repulsion between the molecules indeed does not eliminate the regime of coexistence.

1. The case of bosons with hard core repulsion

In that case we assume that the boson-boson repulsion U' in the lattice case and g_{BB} in the continuum case is going to infinity. Using the Jordan-Wigner transformation [88], one shows that the partition function of these hard core bosons is equal to that of free spinless fermions. At zero temperature, the density of fermionic atoms ρ_F and the density of bosonic molecules ρ_B in the ground state are given by: $\rho_F=N_F/L=2k_F/\pi$ and $\rho_B=N_B/L=k_B/\pi$, where k_F is the Fermi momentum of the atoms and k_B is the Fermi momentum of the spinless fermions (i.e., the pseudo-Fermi momentum of the molecules). The chemical potential satisfies $\mu=\epsilon_F(k_F)=[\nu+\epsilon_B(k_B)]/2$. Up to now, we have not specified the dispersion of the atoms and of the molecules. In the lattice case, these dispersions are obtained from Eq. (2) as $\epsilon_F(k)=-2t\cos(k)$ and $\epsilon_B(k)=-2t'\cos(k)$. As a function of the chemical potential μ three different regimes can be obtained. In the first one, for $-2t<\mu<\nu/2-t'$, only unpaired atoms are present. In the second one for $\nu/2-t'<\mu<2t$, unpaired atoms and molecules coexist. In the last one, for $2t<\mu<\nu 2+t'$, all the available levels of unpaired atoms are filled, and the available levels for molecules are partially filled. As a result, the system behaves as if only molecules were present. This last

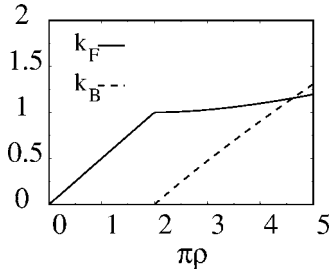

FIG. 1. The behavior of k_F and k_B for positive detuning $\nu>0$ as a function of the total density ρ. For low densities, only atoms are present ($k_B=0$). At higher densities such that $\pi\rho>2\sqrt{m_F\nu}$, a nonzero density of molecules appears. At the critical density, the slopes of k_F and k_B versus ρ are discontinuous. We have taken $m_F\nu=1$.

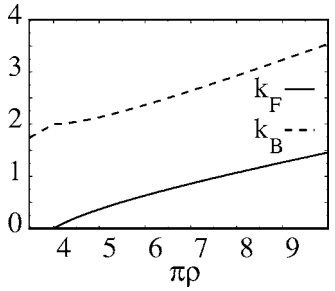

FIG. 2. The behavior of k_F and k_B for negative detuning $\nu<0$. For low densities, only the molecules are present ($k_F=0$). For $\pi\rho>4\sqrt{m_F|\nu|}$, molecules coexist with atoms. At the critical density, the slopes of k_F and k_B versus ρ are discontinuous.

phase is in fact a degenerate Tonks-Girardeau gas of molecules [62,63]. In the intermediate regime, the fermions form a two-component Luttinger liquid [55,56] and the bosons form a single component Luttinger liquid [61]. Similar calculations can be performed in the case of fermions and bosons in the continuum described by Eq. (1). With free fermions and hard core bosons in the continuum the condition on the chemical potential becomes: $k_F^2/2m_F=\mu$ and $k_B^2/4m_F+\nu=2\mu$, with the constraint $(\pi/2)\rho_{\text{tot.}}=(k_F+k_B)$ where $\rho_{\text{tot.}}=2\rho_B+\rho_F$ is the total density of atoms. As a result:

$$k_F=\frac{1}{3}\sqrt{\pi^2\rho^2+12m_F\nu}-\frac{\pi}{6}\rho,$$

$$k_B=\frac{2\pi\rho-\sqrt{\pi^2\rho^2+12m_F\nu}}{3}, \tag{5}$$

and these solutions are physical when they give both $k_F>0$ and $k_B>0$. For $\nu>0$, $k_B>0$ provided $\rho_{\text{tot.}}>\rho^{(1)}_{\text{tot.},c}=(2/\pi)\sqrt{m_F\nu}$. For $\rho<\rho^{(1)}_{\text{tot.},c}$, the density of molecules is vanishing and $\rho_{\text{tot.}}=\rho_F$. Above the critical density $\rho^{(1)}_{\text{tot.},c}$, atoms and molecules coexist. As ρ crosses the critical density, the slope of k_B versus ρ jumps from 0 to $\pi/2$. The Fermi wave vector k_F possesses a similar slope discontinuity at the critical density, with zero slope above the critical density. The behavior of k_F and k_B as a function of the density is represented in Fig. 1.

For $\nu<0$, $k_F>0$ provided $\rho>\rho^{(2)}_{\text{tot.},c}=(4/\pi)\sqrt{m_F|\nu|}$. For $\rho<\rho^{(2)}_{\text{tot.},c}$ the density of unpaired atoms is vanishing, and $\rho=\rho_B$. Above the critical density, atoms and molecules coexist. As before, the slope of the curve k_F versus ρ is discontinuous at the critical density, being zero below and $\pi/3$ above. The behavior of k_F and k_B as a function of the density for $\nu<0$ is represented in Fig. 2.

The slope discontinuities in k_B and k_F have important consequences for the compressibility. Indeed, above the critical density the chemical potential behaves as $O(\rho-\rho_{\text{tot.}c})^2$, so that the compressibility $\chi=(\rho^2(\partial\mu/\partial\rho))^{-1}$ becomes infinite as the critical density is approached from above, signaling a first-order phase transition. Such first order transitions associated with the emptying of a band have been analyzed in the context of Luttinger liquid theory in Refs. [90–92].

2. The case of bosons with finite repulsion

We have seen in the previous section that in the case of hard core repulsion between the molecules, both in the lattice case and in the continuum case, that having $\nu<0$ did not prevent the formation of unpaired atoms provided the total density of atoms was large enough. This was related with the increase of the chemical potential of bosons as a result of repulsion when the density was increased. In this section, we want to analyze a slightly more realistic case where the repulsion between bosons is finite and check that coexistence remains possible. In the lattice case, the problem is tractable only with numerical approaches [93,94]. In the continuum case, however, bosons with contact repulsion are exactly solvable by Bethe ansatz techniques [89]. The density of molecules can therefore be obtained by solving a set of integral equations [89,95]. After having introduced dimensionless variables, they read:

$$2\pi g(x)=1+2\lambda\int_{-1}^{1}\frac{g(y)dy}{\lambda^2+(x-y)^2}, \tag{6}$$

$$\bar{\epsilon}(x)=x^2-1+\frac{\lambda}{\pi}\int_{-1}^{1}dy\bar{\epsilon}(y)\left[\frac{1}{\lambda^2+(x-y)^2}-\frac{1}{\lambda^2+(1-y)^2}\right], \tag{7}$$

$$\mu_B=\nu+\frac{\hbar^2q_0^2}{2m_B}\left[1+\frac{\lambda}{\pi}\int_{-1}^{1}\frac{1}{\lambda^2+(x-1)^2}\bar{\epsilon}(x)dx\right], \tag{8}$$

where

$$g(x)=\rho(q_0x);\quad \lambda=\frac{c}{q_0};\quad \gamma=\frac{c}{\rho_B},\quad c=\frac{m_Bg_{BB}}{\hbar^2}, \tag{9}$$

$$\rho_B=\int_{-q_0}^{q_0}\rho(q)dq, \tag{10}$$

$$\gamma=\frac{c}{\rho_B}, \tag{11}$$

q_0 is a pseudofermion momentum and g_{BB} is the boson-boson interaction defined in Eq. (1). From μ_B, one obtains $\rho_F=(2/\pi)\sqrt{m_F\mu_B}$. Finally, using the definition of the total

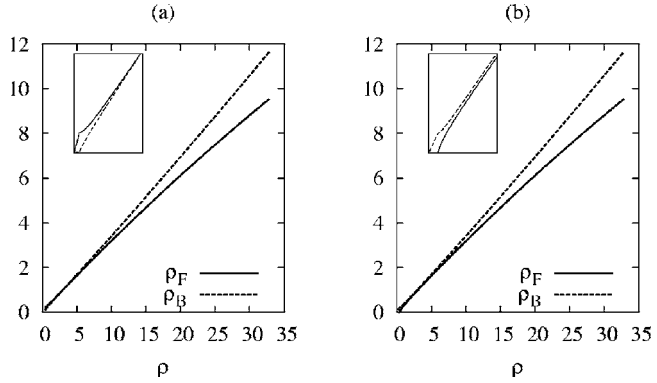

FIG. 3. The density of molecules ρ_B and unpaired atoms ρ_F as a function of the total density ρ. (a) The case of a repulsion $c=100$ and a positive detuning $\nu=0.1$. Inset: the behavior of the boson and fermion densities near the origin. (b) The case of a repulsion $c=100$ and a negative detuning $\nu=-0.1$. Inset: the behavior of the boson and fermion densities near the origin. In both cases, at large total density, the density of molecules is increasing more rapidly than the density of unpaired atoms. At the critical density a cusp is visible in the density of atoms [inset of (a)] for positive ν and in the density of molecules [inset of (b)] for negative ν, as in the case of infinite repulsion between the molecules.

density $\rho=2\rho_B+\rho_F$ one can map the molecule density and the free atom density as a function of the total density of atoms. The resulting equation of state can be written in terms of dimensionless parameters as

$$\frac{\hbar^2\rho_B}{m_B g_{1D}} = \mathcal{F}\left(\frac{\hbar^2\rho}{m_B g_{1D}}, \frac{\hbar^2\nu}{m_F g_{1D}^2}\right). \tag{12}$$

The behavior of the boson density ρ_B and fermion density ρ_F as a function of total density ρ can be understood in qualitative terms. Let us first discuss the case of negative detuning. For sufficiently low densities, only bosons are present. However, in that regime, the boson-boson repulsion is strong, and the boson chemical potential is increasing with the boson density. As a result, when the density exceeds a critical density ρ_c, the fermion chemical potential becomes positive, and the density of fermions becomes nonzero. The appearance of fermions is causing a cusp in the boson density plotted versus the total density. When the density of particles becomes higher, the boson-boson interaction becomes weaker, and the boson chemical potential barely increases with the density. As a result, the fermion density becomes almost independent of the total density. In the case of positive detuning, for low density, only fermions are present. Again, the increase of fermion density results in an increase of chemical potential and above a certain threshold in fermion density, bosons start to appear, creating a cusp in the dependence of the fermion density upon the total density. At large density, the detuning becomes irrelevant, and the fermion density barely increases with the total density.

To illustrate this behavior, we have solved numerically the integral equations (6), and calculated the resulting fermion and boson densities. A plot of the density of bosons as well as the density of fermions for $\nu>0$ and for $\nu<0$ is shown in Fig. 3. The slope discontinuities at the critical density remain visible. This implies that the divergence of the compressibility at the critical density remains when the repulsion between the molecules becomes finite.

We have thus seen that generally we should expect a coexistence of fermionic atoms and bosonic molecules provided the repulsion between the molecules is sufficiently strong. The repulsion between the molecules also results in a nonzero velocity for sound excitations in the molecule Bose gas. Thus, this gas will behave as a Luttinger liquid, and the unpaired atoms will form another Luttinger liquid. The treatment of the present section thus leads us to the prediction of two decoupled Luttinger liquids describing the molecular and the atomic gas. However, this treatment assumed that the term converting atoms into molecules was so small that it did not affect significantly the spectrum of the system. In the following, we will treat the effect of a small but not infinitesimal conversion term in Eqs. (2) and (1) using bosonization techniques. We will show that the conversion term can lead to phase coherence between the atoms and the molecules, and we will discuss the properties of the phase in which such coherence is observed.

III. PHASE DIAGRAM AND CORRELATION FUNCTIONS

A. Derivation of the bosonized Hamiltonian

In this section, we consider the case discussed in Sec. II where neither the density of molecules nor the density of atoms vanishes. As discussed in Sec. II, this requires a sufficiently large initial density of atoms. As there is both a nonzero density of atoms and of molecules, they both form Luttinger liquids [55,56,61]. These Luttinger liquids are coupled by the repulsion between atoms and molecules V_{BF} and via the conversion term or Josephson coupling λ. To describe these coupled Luttinger liquids, we apply bosonization [54] to the Hamiltonians (2) and (1). For the sake of definiteness, we discuss the bosonization procedure in detail only in the case of the continuum Hamiltonian (1). For the lattice Hamiltonian (2), the steps to follow are identical provided the system is not at a commensurate filling. At commensurate filling, umklapp terms must be added to the bosonized Hamiltonian and can result in Mott phases [54]. This case is treated in Sec. IV.

To derive the bosonized Hamiltonian describing the low-energy spectrum of the Hamiltonian (1), we need first to consider the bosonized description of the system when all atom-molecule interactions are turned off. For $\lambda=0$, $V_{BF}=0$, both N_f and N_b are conserved and the bosonized Hamiltonian equivalent to (2) and (1) is given by

$$H = H_b + H_\rho + H_\sigma,$$

$$H_b = \int \frac{dx}{2\pi}\left[u_b K_b(\pi\Pi_b)^2 + \frac{u_b}{K_b}(\partial_x\phi_b)^2\right],$$

$$H_\rho = \int \frac{dx}{2\pi}\left[u_\rho K_\rho(\pi\Pi_\rho)^2 + \frac{u_\rho}{K_\rho}(\partial_x\phi_\rho)^2\right],$$

$$H_\sigma = \int \frac{dx}{2\pi}\left[u_\sigma K_\sigma(\pi\Pi_\sigma)^2 + \frac{u_\sigma}{K_\sigma}(\partial_x\phi_\sigma)^2\right] - \frac{2g_{1\perp}}{(2\pi\alpha)^2}\int dx \cos\sqrt{8}\phi_\sigma, \quad (13)$$

where $[\phi_\nu(x),\Pi_{\nu'}(x')]=i\delta(x-x')\delta_{\nu,\nu'}$, $(\nu,\nu'=b,\sigma,\rho)$. In the context of cold atoms, the Hamiltonian (13) has been discussed in Refs. [55,56,61]. The parameters K_ρ, the Luttinger exponent, and u_ρ, u_σ, the charge and spin velocities, are known functions of the interactions [72,96–98], with $K_\rho=1$ in the noninteracting case, $g_{1\perp}$ is a marginally irrelevant interaction, and at the fixed point of the RG flow $K_\sigma^*=1$. For the bosonic system, the parameters u_b, K_b can be obtained from numerical calculations [94] in the lattice case or from the solution of the Lieb-Liniger model [89] in the continuum case. In the case of noninteracting bosons $K_b\to\infty$ and in the case of hard core bosons $K_b=1$ [60,62,63]. An important property of the parameters K_b and K_ρ is that they decrease as (respectively) the boson-boson and fermion-fermion interaction become more repulsive. The bosonized Hamiltonian (13) is also valid in the lattice case (2) provided that both N_f and N_b do not correspond to any commensurate filling.

The fermion operators can be expressed as functions of the bosonic fields appearing in Eq. (13) as [54]

$$\psi_\sigma(x) = \sum_{r=\pm} e^{irk_F n\alpha}\psi_{r,\sigma}(x=n\alpha), \quad (14)$$

$$\psi_{r,\sigma}(x) = \frac{e^{i/\sqrt{2}[\theta_\rho - r\phi_\rho + \sigma(\theta_\sigma - r\phi_\sigma)](x)}}{\sqrt{2\pi\alpha}}, \quad (15)$$

where the index $r=\pm$ indicates the right/left movers, α is a cutoff equal to the lattice spacing in the case of the model Eq. (2). Similarly, the boson operators are expressed as [54]

$$\frac{b_n}{\sqrt{\alpha}} = \Psi_b(x=n\alpha), \quad (16)$$

$$\Psi_b(x) = \frac{e^{i\theta_b}}{\sqrt{2\pi\alpha}}[1 + A\cos(2\phi_b - 2k_B x)]. \quad (17)$$

In Eqs. (14)–(16), we have introduced the dual fields [54] $\theta_\nu(x)=\pi\int^x\Pi_\nu(x')dx'$ $(\nu=\rho,\sigma,b)$, $k_F=\pi N_f/2L$, and $k_B=\pi N_b/L$ where L is the length of the system. The fermion density is given by [54]

$$\sum_\sigma \frac{n_{f,n,\sigma}}{\alpha} = \rho_f(x=n\alpha) = -\frac{\sqrt{2}}{\pi}\partial_x\phi_\rho + \frac{\cos(2k_F x - \sqrt{2}\phi_\rho)}{\pi\alpha}\cos\sqrt{2}\phi_\sigma, \quad (18)$$

and the boson density by [54]

$$\frac{n_{b,n}}{a} = \rho_b(x) = -\frac{1}{\pi}\partial_x\phi_b + \frac{\cos(2k_B x - 2\phi_b)}{\pi\alpha}. \quad (19)$$

The detuning term in Eq. (1) is thus expressed as

$$H_{\text{detuning}} = -\frac{\nu}{\pi}\int dx\partial_x\phi_b. \quad (20)$$

We now turn on a small λ and a small V_{BF}. The effect of a small V_{BF} on a boson-fermion mixture has been investigated previously [99,100]. The forward scattering contribution is

$$\frac{V_{BF}\sqrt{2}}{\pi^2}\int dx\ \partial_x\phi_b\partial_x\phi_\rho, \quad (21)$$

and as discussed in Ref. [99], it can give rise to a phase separation between bosons and fermions if it is too repulsive. Otherwise, it only leads to a renormalization of the Luttinger exponents. The atom molecule repulsion term also gives a backscattering contribution:

$$\frac{2V_{BF}}{(2\pi\alpha)^2}\int dx\cos[2\phi_b - \sqrt{2}\phi_\rho - 2(k_F - k_B)x]\cos\sqrt{2}\phi_\sigma, \quad (22)$$

however in the general case, $k_F\neq k_B$ this contribution is vanishing. In the special case of $k_B=k_F$, the backscattering can result in the formation of a charge density wave. This effect will be discussed in Sec. III B 3. The contribution of the λ term is more interesting [78,79]. Using Eqs. (14)–(16), we find that the most relevant contribution reads:

$$H_{bf} = \frac{2\lambda}{\sqrt{2\pi^3\alpha^3}}\int dx\cos(\theta_b - \sqrt{2}\theta_\rho)\cos\sqrt{2}\phi_\sigma. \quad (23)$$

In the next section, we will see that this term gives rise to a phase with atom-molecule coherence when the repulsion is not too strong.

B. Phase diagram

1. Phase with atom-molecule coherence

The effect of the term (23) on the phase diagram can be studied by renormalization group techniques [54]. A detailed study of the renormalization group equations has been published in Ref. [78]. Here, we present a simplified analysis, which is sufficient to predict the phases that can be obtained in our system. The scaling dimension of the boson-fermion coupling term (23) is: $1/4K_b+1/2K_\rho+\frac{1}{2}K_\sigma$. For small λ it is reasonable to replace K_σ with its fixed point value $K_\sigma^*=1$. Therefore, the RG equation for the dimensionless coupling $\tilde{\lambda}=\lambda\alpha^{1/2}/u$ (where u is one of the velocities u_ρ, u_σ, u_b) reads:

$$\frac{d\tilde{\lambda}}{d\ell} = \left(\frac{3}{2} - \frac{1}{2K_\rho} - \frac{1}{4K_b}\right)\tilde{\lambda}, \quad (24)$$

where ℓ is related to the renormalized cutoff $\alpha(\ell)=\alpha e^\ell$. We thus see that for $1/2K_\rho+1/4K_b<3/2$, this interaction is relevant. Since for hardcore bosons [62,63] $K_b=1$ and for noninteracting bosons $K_b=\infty$, while for free fermions $K_\rho=1$ and in the lattice case for $U=\infty$ one has $K_\rho=1/2$ [98], we see that the inequality is satisfied unless there are very strongly repulsive interactions both in the boson system and in the fermion system. When this inequality is not satisfied, for instance in the case of fermions with nearest-neighbor repulsion [101,102], in which one can have $1/4<K_\rho<1/2$ and hardcore bosons with nearest neighbor repulsion

[58,103], in which one can have $K_b=1/2$, the atoms and the molecules decouple. This case is analogous to that of the mixture of bosons and fermions [99,100] and charge density waves can be formed if k_B and k_F are commensurate. The phase transition between this decoupled phase and the coupled phase belongs to the Berezinskii-Kosterlitz-Thouless (BKT) universality class [104]. As pointed out in Ref. [78], in the decoupled phase, the effective interaction between the fermions can be attractive. In that case, a spin gap is formed [54,59] and the fermions are in a Luther-Emery liquid state with gapless density excitations. Let us consider the coupled phase in more detail. The relevance of the interaction (23) leads to the locking of ϕ_σ, i.e., it results in the formation of a spin gap. To understand the effect of the term $\cos(\theta_b - \sqrt{2}\theta_\rho)$, it is better to perform a rotation:

$$\begin{pmatrix} \theta_- \\ \theta_+ \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{3}} & -\frac{\sqrt{2}}{\sqrt{3}} \\ \frac{\sqrt{2}}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} \theta_b \\ \theta_\rho \end{pmatrix}, \tag{25}$$

and the same transformation for the ϕ_ν. This transformation preserves the canonical commutation relations between $\phi_\pm$ and $\Pi_\pm$. Under this transformation, H_b+H_ρ becomes

$$H_b + H_\rho = \int \frac{dx}{2\pi} \sum_{\nu=\pm} \left[u_\nu K_\nu (\pi \Pi_\nu)^2 + \frac{u_\nu}{K_\nu} (\partial_x \phi_\nu)^2 \right] + \int \frac{dx}{2\pi} [g_1 (\pi\Pi_+)(\pi\Pi_-) + g_2 \partial_x \phi_+ \partial_x \phi_-], \tag{26}$$

where the coefficients $u_\pm$, $K_\pm$, $g_{1,2}$ can be found in Appendix A. The boson-fermion conversion term H_{bf} defined in Eq. (23) becomes

$$H_{bf} = \frac{\lambda}{\sqrt{2\pi^3}\alpha} \int dx \cos\sqrt{3}\theta_- \cos\sqrt{2}\phi_\sigma. \tag{27}$$

After the rotation, we see that when λ is relevant, the field θ_- is also locked, but ϕ_+ remains gapless. Since the field θ_- is the difference of the superfluid phase of the atoms and the one of the molecules, this means that when λ becomes relevant, unpaired atoms and molecules share the same superfluid phase, i.e., they become coherent. The gap induced by the term λ can be estimated from the renormalization group equation (24). Under the renormalization group, the dimensionless parameter $\tilde{\lambda}(\ell)$ grows until it becomes of order one at a scale $\ell=\ell^*$ where the perturbative approach breaks down. Beyond the scale ℓ^*, the fields θ_- and ϕ_σ behave as classical fields. Therefore, the associated energy scale $u/(\alpha e^{\ell^*})$ is the scale of the gap. From this argument, we obtain that the gap behaves as

$$\Delta \sim \frac{u}{\alpha} \left(\frac{\lambda \alpha^{1/2}}{u} \right)^{1/(3/2-1/2K_\rho-1/4K_b)}. \tag{28}$$

The gapful excitations have a dispersion $\epsilon(k)=\sqrt{(uk)^2+\Delta^2}$ and are kinks and antikinks of the fields θ_- and ϕ_σ [105]. More precisely, since a kink must interpolate between degenerate classical ground states of the potential (27), we find that when a kink is present $\theta_-(+\infty)-\theta_-(-\infty)=\pm\pi/\sqrt{3}$ and $\phi_\sigma(+\infty)-\phi_\sigma(-\infty)=\pi/\sqrt{2}$. This indicates that a kink is carrying a spin 1/2, and is making the phase θ_b of the bosons jump by $\pi/3$ and the phase of the superfluid order parameter $\sqrt{2}\theta_\rho$ of the fermions jump by $-2\pi/3$. Since the current of bosons is $j_b=u_bK_b\pi\Pi_b=u_bK_b\partial_x\theta_b$ and the current of fermions is $j_F=\sqrt{2}u_\rho K_\rho \pi\Pi_\rho=\sqrt{2}u_\rho K_\rho \partial_x\theta_\rho$, this indicates that counterpropagating supercurrents of atoms and molecules exist in the vicinity of the kinks. Therefore, we can view the kinks and antikinks as composite objects formed of vortices bound with a spin 1/2. We note that the kinks and antikinks may not exhaust all the possible gapful excitations of the system. In particular, bound states of kinks and antikinks, known as breathers, may also be present [105]. However, these gapful excitations present a larger gap than the single kinks. Let us now turn to the gapless field ϕ_+. This field has a simple physical interpretation. Considering the integral

$$-\frac{1}{\pi}\int_{-\infty}^{\infty} dx \partial_x \phi_+ = -\frac{1}{\pi\sqrt{3}} \int_{-\infty}^{\infty} dx \partial_x (\sqrt{2}\phi_b + \phi_\rho) = \frac{\mathcal{N}}{\sqrt{6}}, \tag{29}$$

showing that $\phi_+(\infty)-\phi_+(-\infty)$ measures the total number of particles in the system $\mathcal{N}$. Thus (Π_+, ϕ_+) describe the total density excitations of the system.

The resulting low-energy Hamiltonian describing the gapless total density modes reads:

$$H_+ = \int \frac{dx}{2\pi} \left[u_+^* K_+^* (\pi\Pi_+)^2 + \frac{u_+^*}{K_+^*} (\partial_x \phi_+)^2 \right], \tag{30}$$

where u_+^*, K_+^* denote renormalized values of u_+, K_+. This renormalization is caused by the residual interactions between gapless modes and the gapped modes measured by g_1, g_2 in Eq. (26). Since ϕ_+ measures the total density, the Hamiltonian (30) describes the propagation of sound modes in the 1D fluid with dispersion $\omega(k)=u|k|$. We note than in Refs. [81,106], dispersion relations similar to ours were derived for the sound modes and the superfluid phase difference modes using different methods.

2. Effect of the detuning and applied magnetic field

Having understood the nature of the ground state and the low excited states when λ is relevant we turn to the effect of the detuning term. Equations (20) and (25) show that the detuning term can be expressed as a function of ϕ_+, ϕ_- as

$$H_{\text{detun.}} = -\frac{\nu}{\pi} \int \partial_x \left(\sqrt{\frac{2}{3}}\phi_+ + \frac{\phi_-}{\sqrt{3}} \right). \tag{31}$$

This shows that the detuning does not affect the boson-fermion coupling (23) since it can be eliminated from the Hamiltonian by a canonical transformation $\phi_\pm \to \phi_\pm + \lambda_\pm x$, where $\lambda_+=\nu\sqrt{(2/3)}$ and $\lambda_-=\nu/\sqrt{3}$. For a fixed total density, changing the detuning only modifies the wave vectors k_B and k_F. As discussed extensively in Sec. II B, for a detuning sufficiently large in absolute value, only molecules or only at-

oms are present, and near the critical value of the detuning, the compressibility of the system is divergent. We therefore conclude that in one dimension, the crossover from the Bose condensation to the superfluid state, as the detuning is varied, is the result of the band-filling transitions at which either the density of the atoms or the molecules goes to zero. At such band filling transitions, $v_{\rho,\sigma} \to 0$ (respectively, $v_b \to 0$) and bosonization breaks down [90–92]. The cases where only the molecules or only the atoms are present have been analyzed in Ref. [76]. Moreover, it was shown that in the case of a broad Fano-Feshbach resonance, the zone of coexistence becomes very narrow [76]. In the narrow Fano-Feshbach resonance case we are investigating, the zone of coexistence can be quite important.

Application of a magnetic field can also induce some phase transitions. The interaction with the magnetic field reads

$$H_{\text{magn}} = -\frac{h}{\pi\sqrt{2}} \int dx \partial_x \phi_\sigma. \tag{32}$$

The effect of the magnetic field is to lower the gap for the creation of kink excitations (remember that they carry a spin 1/2). As a result, when it becomes larger than the gap, the magnetic field induces a commensurate incommensurate transition [107–110] that destroys the coherence between atoms and molecules and gives back decoupled Luttinger liquids [111]. In that regime, the behavior of the system is described by the models of Refs. [99,100]. Commensurate-incommensurate transitions have already been discussed in the context of cold atoms in Ref. [112]. In the problem we are considering, however, since two fields are becoming gapless at the same time, θ_- and ϕ_σ, there are some differences [113,114] from the standard case [112], in particular the exponents at the transition are nonuniversal.

To conclude this section, we notice that we have found three types of phase transitions in the system we are considering. We can have Kosterlitz-Thouless phase transitions as a function of interactions, where we go from a phase with locked superfluid phases between the bosons and the fermions at weak repulsion to a phase with decoupled bosons and fermions at strong repulsion. We can have band-filling transitions as a function of the detuning between the phase in which atoms and molecule coexist and phases where only atoms or only molecules are present. Finally, we can have commensurate-incommensurate transitions as a function of the strength of the magnetic field. In the following section, we discuss the correlation functions of superfluid and charge density wave order parameters in the phase in which molecules and atoms coexist with their relative superfluid phase θ_- locked.

3. Quantum Ising phase transition for $k_F = k_B$

In the case of $k_F = k_B$, the backscattering term (22) is nonvanishing. This term induces a mutual locking of the densities of the bosons and the fermions [99] and favors charge density wave fluctuations. This term is competing with the Josephson term (23) which tends to reduce density wave fluctuations. For $k_F = k_B$ the relevant part of the Hamiltonian given by the combination of the terms (22) and (23) reads

$$H_{\text{Josephson+CDW Lock.}} = \int dx \left[\frac{2\lambda}{\sqrt{2\pi^3\alpha^3}} \cos(\theta_b - \sqrt{2}\theta_\rho) + \frac{2V_{BF}}{(2\pi\alpha)^2} \cos(2\phi_b - \sqrt{2}\phi_\rho) \right] \cos\sqrt{2}\phi_\sigma. \tag{33}$$

Using a transformation $\phi_b = \tilde{\phi}_b/\sqrt{2}$, $\theta_b = \tilde{\theta}_b\sqrt{2}$, and introducing the linear combinations

$$\phi_1 = \frac{\tilde{\phi}_b + \phi_\rho}{\sqrt{2}}, \tag{34}$$

$$\phi_2 = \frac{\tilde{\phi}_b - \phi_\rho}{\sqrt{2}} \tag{35}$$

and similar combinations for the dual fields, we can rewrite the interaction term (33) as

$$H_{\text{Josephson+CDW Lock.}} = \int dx \left[\frac{2\lambda}{\sqrt{2\pi^3\alpha^3}} \cos 2\theta_2 + \frac{2V_{BF}}{(2\pi\alpha)^2} \cos 2\phi_2 \right] \cos\sqrt{2}\phi_\sigma. \tag{36}$$

From this Hamiltonian, it is immediate to see that a quantum Ising phase transition occurs between the density wave phase ϕ_2 and the superfluid phase θ_2 at a critical point $\lambda_c = V_{BF}/\sqrt{8\pi\alpha}$ [115–117]. Indeed, the field ϕ_σ being locked, we can replace $\cos\sqrt{2}\phi_\sigma$ by its expectation value in Eq. (36), and rewrite (36) as a free massive Majorana fermions Hamiltonian [115–117]. At the point λ_c, the mass of one of these Majorana fermions vanishes giving a quantum critical point in the Ising universality class [118]. On one side of the transition, when $\lambda > \lambda_c$, the system is in the superfluid state discussed in Sec. III B, on the other side $\lambda < \lambda_c$, the charge density wave state discussed in Ref. [99] is recovered.

C. Correlation functions

In order to better characterize the phase in which λ is relevant, we need to study the correlation function of the superfluid and the charge density wave operators. Let us begin by characterizing the superfluid order parameters. First, let us consider the order parameter for BEC of the molecules. As a result of the locking of the fields θ_- and ϕ_σ, the boson operator Eq. (16) becomes at low energy

$$\Psi_B(x) \sim \frac{e^{i\sqrt{(2/3)}\theta_+}}{\sqrt{2\pi\alpha}} \langle e^{-i\theta_-/\sqrt{3}} \rangle. \tag{37}$$

An order of magnitude of $\langle e^{-i\theta_-/\sqrt{3}} \rangle$ can be obtained from a scaling argument similar to the one giving the gap. Since the scaling dimension of the field $e^{-i\theta_-/\sqrt{3}}$ is $1/12K_-$, and since the only length scale in the problem is e^{ℓ^*}, we must have $\langle e^{-i\theta_-/\sqrt{3}} \rangle \sim e^{-\ell^*/12K_-} \sim (\lambda\alpha^{1/2}/u)^{1/12K_-}$. Similarly, the order pa-

rameter for s-wave superconductivity of the atoms $O_{SS} = \Sigma_\sigma \psi_{r,\sigma}\psi_{-r,-\sigma}$ becomes

$$O_{SS} = \frac{e^{i\sqrt{2}\theta_\rho}}{\pi\alpha}\cos\sqrt{2}\phi_\sigma \sim \frac{e^{i\sqrt{(2/3)}\theta_+}}{\pi\alpha}\langle e^{2i/\sqrt{3}\theta_-}\cos\sqrt{2}\phi_\sigma\rangle, \tag{38}$$

thus indicating that the order parameters of the BEC and the BCS superfluidity have become identical in the low energy limit [32,33]. This is the signature of the coherence between the atom and the molecular superfluids. The boson correlator behaves as

$$\langle \Psi_B(x,\tau)\Psi_B(0,0)\rangle \sim \left(\frac{\alpha^2}{x^2+(u\tau)^2}\right)^{1/6K_+}. \tag{39}$$

As a result, the molecule momentum distribution becomes $n_B(k) \sim |k|^{1/(3K_+)-1}$. One can see that the tendency toward superfluidity is strongly enhanced since the divergence of $n_B(k)$ for $k \to 0$ is increased by the coherence between the molecules and the atoms. This boson momentum distribution can, in principle, be measured in a condensate expansion experiment [119,120].

Having seen that superfluidity is enhanced in the system, with BEC and BCS order parameters becoming identical, let us turn to the density wave order parameters. These order parameters are simply the staggered components of the atom and molecule density in Eqs. (18) and (19). In terms of $\phi_\pm$, the staggered component of the molecule density is reexpressed as

$$\rho_{2k_B,b}(x) \sim \cos\left[2\left(\frac{\phi_-}{\sqrt{3}}+\frac{\sqrt{2}}{\sqrt{3}}\phi_+\right)-2k_b x\right], \tag{40}$$

and the staggered component of the fermion density as

$$\rho_{2k_F,f}(x) \sim \cos\left[\sqrt{2}\left(-\frac{\sqrt{2}}{\sqrt{3}}\phi_-+\frac{1}{\sqrt{3}}\phi_+\right)-2k_F x\right], \tag{41}$$

where we have taken into account the long range ordering of ϕ_σ. We see that the correlations of both $\rho_{2k_B,b}(x)$ and $\rho_{2k_F,f}(x)$ decay exponentially due to the presence of the disorder field ϕ_- dual to θ_-. In more physical terms, the exponential decay of the density-wave correlations in the system results from the constant conversion of molecules into atoms and the reciprocal process which prevents the buildup of a well-defined atomic Fermi-surface or molecule pseudo-Fermi surface. The exponential decay of the density wave correlations in this system must be contrasted with the power-law decay of these correlations in a system with only bosons or in a system of fermions with attractive interactions [54]. In fact, if we consider that our new particles are created by the operator $\psi_b \sim \psi_\uparrow\psi_\downarrow$, we can derive an expression of the density operators of these new particles by considering the product $\psi_b\psi_\uparrow\psi_\downarrow$. Using the Haldane expansion of the boson creation and annihilation operators [60], we can write this product as

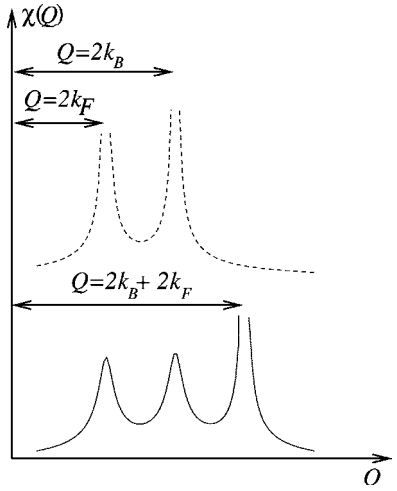

FIG. 4. Fourier transform of the static density density correlations. In the decoupled phase (dashed line), two peaks are obtained at twice the Fermi wave vector of the unpaired atoms and at twice the pseudo-Fermi wave vector of the molecules. In the coupled phase (solid line), the peaks are replaced by maxima at $Q=2k_F$ and $Q=2k_B$. A new peak at $Q=2(k_F+k_B)$ is obtained as a result of boson-fermion coherence.

$$\begin{aligned}\psi_b^\dagger\psi_\uparrow\psi_\downarrow &\sim e^{-i\theta_b}\left[\sum_{m=0}^{\infty}\cos(2m\phi-2mk_B x)\right]\\ &\times e^{i\sqrt{2}\theta_\rho}[\cos\sqrt{2}\phi_\sigma+\cos(\sqrt{2}\phi_\rho-2k_F x)]\\ &\sim \langle e^{-i(\theta_b-\sqrt{2}\theta_\rho)}\cos\sqrt{2}\phi_\sigma\rangle\cos(\sqrt{6}\phi_+-2(k_F+k_B)x),\end{aligned} \tag{42}$$

where $(k_F+k_B)=\pi(2N_b+N_f)/2L=\pi\rho_{\text{pairs}}$ can be interpreted as the pseudo-Fermi wave vector of composite bosons. As a result, when there is coherence between atoms and molecule, power-law correlations appear in the density-density correlator near the wave vector $2k_F+2k_B$ and the intensity of these correlations is proportional to the $|\langle e^{-i(\theta_b-\sqrt{2}\theta_\rho)}\cos\sqrt{2}\phi_\sigma\rangle|^2$. The resulting behavior of the Fourier transform of the density-density correlator is represented in Fig. 4.

Another interesting consequence of the existence of atom/molecule coherence is the possibility of having nonvanishing cross correlations of the atom and the molecule density. In the three-dimensional case such cross correlations have been studied in Ref. [121]. If we first consider cross correlations $\langle T_\tau\rho_{2k_B,b}(x,\tau)\rho_{2k_F,f}(0,0)\rangle$ we notice that due to the presence of different exponentials of ϕ_+ in Eqs. (40) and (41), this correlator vanishes exactly. Therefore, no cross correlation exists between the staggered densities. However, if we consider the cross correlations of the uniform densities, we note that since they can all be expressed as functions of $\partial_x\phi_+, \partial_x\phi_-$, such cross correlations will be nonvanishing. More precisely, since

$$\rho_F = -\frac{\sqrt{2}}{\pi\sqrt{3}}\partial_x\phi_+ + \frac{2}{\pi\sqrt{3}}\partial_x\phi_-, \tag{43}$$

$$\rho_B = -\frac{\sqrt{2}}{\pi\sqrt{3}}\partial_x\phi_+ - \frac{1}{\pi\sqrt{3}}\partial_x\phi_-, \tag{44}$$

at low energy we have: $\rho_F \sim \rho_B \sim -(\sqrt{2}/\pi\sqrt{3})\partial_x\phi_+$ and $\langle\rho_F(x)\rho_B(0)\rangle \sim \alpha^2/x^2$.

D. The Luther Emery point

In this section, we will obtain detailed expressions for these correlation functions at a special exactly solvable point of the parameter space. At this point, the kinks of the fields ϕ_σ and θ_- become free massive fermions. This property, and the equivalence of free massive fermions in 1D with the two-dimensional noncritical Ising model [122–127] allows one to find exactly the correlation functions.

1. Mapping on free fermions

As we have seen, after the rotation (25), if we neglect the interaction terms of the form $\Pi_+\Pi_-$ or $\partial_x\phi_+\partial_x\phi_-$, the Hamiltonian of the massive modes ϕ_-, ϕ_σ can be rewritten as

$$\begin{aligned} H = &\int \frac{dx}{2\pi}\left[u_\sigma^* K_\sigma^* (\pi\Pi_\sigma)^2 + \frac{u_\sigma^*}{K_\sigma^*}(\partial_x\phi_\sigma)^2\right] \\ &+ \int \frac{dx}{2\pi}\left[u_- K_- (\pi\Pi_-)^2 + \frac{u_-}{K_-}(\partial_x\phi_-)^2\right] \\ &+ \frac{\lambda}{\sqrt{2\pi^3\alpha^3}}\int dx \cos\sqrt{3}\theta_- \cos\sqrt{2}\phi_\sigma, \end{aligned} \tag{45}$$

where $K_\sigma^*=1$. When the Luttinger exponent is $K_-=3/2$, it is convenient to introduce the field $\bar{\phi}=\sqrt{(3/2)}\theta_-$ and its dual, $\bar{\theta}=\sqrt{(2/3)}\phi_-$, and rewrite the Hamiltonian (45) as

$$\begin{aligned} H = &\int \frac{dx}{2\pi}[u_\sigma^*(\pi\Pi_\sigma)^2 + u_\sigma^*(\partial_x\phi_\sigma)^2] + \int \frac{dx}{2\pi}[u_-(\pi\bar{\Pi})^2 \\ &+ u_-(\partial_x\bar{\phi})^2] + \frac{\lambda}{\sqrt{2\pi^3\alpha}}\int dx \cos\sqrt{2}\bar{\phi}\cos\sqrt{2}\phi_\sigma. \end{aligned} \tag{46}$$

If we neglect the velocity difference, i.e., assume that $u_\sigma^* = u_- = u$, and introduce the pseudofermion fields:

$$\Psi_{r,\sigma} = \frac{e^{(i/\sqrt{2})[(\bar{\theta}-r\bar{\phi})+\sigma(\theta_\sigma - r\phi_\sigma)]}}{\sqrt{2\pi\alpha}} = \frac{e^{i(\Theta_\sigma - r\Phi_\sigma)}}{\sqrt{2\pi\alpha}}, \tag{47}$$

we see immediately that the Hamiltonian (46) is the bosonized form of the following free fermion Hamiltonian:

$$H = \sum_\sigma \int dx\left[-iu\sum_{r=\pm} r\Psi_{r,\sigma}^\dagger \partial_x \Psi_{r,\sigma} + \frac{\lambda}{\sqrt{2\pi\alpha}}\Psi_{r,\sigma}^\dagger \Psi_{r,\sigma}\right]. \tag{48}$$

As a result, for the special value of $K_-=3/2$, the excitations can be described as massive free fermions with dispersion $\epsilon(k)=\sqrt{(uk)^2+m^2}$, where $m=|\lambda|/\sqrt{2\pi\alpha}$. This is known as Luther-Emery solution [59,128]. One can see that the fermions carry a spin 1/2 and a jump of the phase θ_- equal to $\pi/\sqrt{3}$. Therefore they can be identified to the kinks obtained in the semiclassical treatment of Sec. III B. Also, making all velocities equal and $V_{BF}=0$ in Eq. (A1), we find the relation $3/K_- = 1/K_b + 2/K_\rho$ and thus the gap given by the RG varies as $\Delta \sim (u/\alpha)(\lambda\alpha^{1/2}/u)^{1/(3/2-3/4K_-)}$. For $K_-=3/2$ this expression reduces to the one given by the fermion mapping.

2. Density-density correlation functions

To obtain the density-density correlation functions of the atoms and of the molecules at the Luther-Emery point, we have to express the alternating components of the atom and molecule density in terms of the field ϕ_+ and the pseudofermion fields. The fermion density $\rho_{2k_F,f}(x)$ is readily expressed in terms of these fields:

$$\rho_{2k_F,f}(x) = e^{i[\sqrt{(2/3)}\phi_+ - 2k_F x]}(\Psi_{-,\uparrow}^\dagger \Psi_{+,\downarrow}^\dagger + \Psi_{+,\uparrow}^\dagger \Psi_{-,\downarrow}^\dagger) + \text{H.c.}, \tag{49}$$

which enables us to find exactly its correlation functions. In real space, the alternating density density correlation function of the unpaired atoms reads

$$\begin{aligned} &\langle T_\tau \rho_{2k_F,f}(x,\tau)\rho_{-2k_F,f}(0,0)\rangle \\ &= 2\left(\frac{m}{2\pi u}\right)^2\left(\frac{\alpha^2}{x^2+(u\tau)^2}\right)^{K_+/6} \\ &\times\left[K_0^2\left(m\sqrt{\tau^2+\left(\frac{x}{u}\right)^2}\right) + K_1^2\left(m\sqrt{\tau^2+\left(\frac{x}{u}\right)^2}\right)\right], \end{aligned} \tag{50}$$

where K_0 and K_1 are modified Bessel functions [129]. At long distances, expression (50) decays exponentially, with a correlation length $u/m=\xi$, as expected from the general discussion of Sec. III C.

The calculation of the correlation functions of the alternating component of the boson density, $\rho_{2k_B,b}$ is more involved. First, this component can be rewritten in terms of the fields $\Theta_{\uparrow/\downarrow}$ from Eq. (47) as

$$\rho_{2k_B,b}(x) = e^{i[\sqrt{(8/3)}\phi_+ - 2k_B x]}e^{i(\Theta_\uparrow + \Theta_\downarrow)} + \text{H.c.} \tag{51}$$

This expression cannot be written directly in terms of the pseudofermion fields (47) as it is nonlocal with respect to them. However, to obtain the correlation functions of $\rho_{2k_B,b}$, we can use a well-known mapping of Dirac fermions in (1+1) dimensions onto the noncritical two-dimensional Ising model [122–127]. Using this mapping, the fields $e^{i\Theta_\sigma}$ can be reexpressed in terms of the order and disorder parameters of four noncritical two-dimensional Ising models, respectively denoted by $\sigma_{1,2,3,4}$ and $\mu_{1,2,3,4}$. This leads to the following expression for $\rho_{2k_B,b}$:

$$\rho_{2k_B,b} = e^{i[\sqrt{(8/3)}\phi_+ - 2k_B x]}(\sigma_1\mu_2 + i\mu_1\sigma_2)(\sigma_3\mu_4 + i\mu_3\sigma_4) + \text{H.c.}, \tag{52}$$

yielding:

$$\langle T_\tau \rho_{2k_B,b}(x,\tau)\rho_{2k_B,b}(0,0)\rangle \sim \left(\frac{\alpha^2}{x^2+(u\tau)^2}\right)^{2K_+/3} 4\langle\sigma(x,\tau)\sigma(0,0)\rangle^2\langle\mu(x,\tau)\mu(0,0)\rangle^2, \tag{53}$$

where we have used $\langle\sigma_i(x,\tau)\sigma_j(0,0)\rangle=\delta_{ij}\langle\sigma(x,\tau)\sigma(0,0)\rangle$ $(i,j=1,2,3,4)$ and a similar relation for the disorder operators μ_i. The exact correlation functions $\langle\sigma(x,\tau)\sigma(0,0)\rangle$ have been obtained in Ref. [130], in terms of Painlevé III transcendants [131]. The correlation functions of the disorder operators are immediately deduced from these by using the Kramers-Wannier duality. Since we are interested in the low-energy, long-distance properties of the system, it is enough to replace the Painlevé transcendants with their approximation in terms of modified Bessel functions. Then, one finds

$$\langle T_\tau \rho_{2k_B,b}(x,\tau)\rho_{2k_B,b}(0,0)\rangle \sim \left(\frac{\alpha^2}{x^2+(u\tau)^2}\right)^{2K_+/3} K_0^2\left(m\sqrt{\tau^2+\left(\frac{x}{u}\right)^2}\right). \tag{54}$$

The structure factors are the Fourier transform of the Matsubara space density-density response functions (50) and (54). They are obtained from the integrals derived in Appendix B. The response functions are then obtained by the substitution $i\omega\to\omega+i0$, and their imaginary parts yield the scattering cross sections.

With the approximation (54), the bosonic structure factor is

$$\chi^B_{\rho\rho}(\pm 2k_B+q,\omega)=\frac{2\pi}{u}\left(\frac{m\alpha}{u}\right)^{4K_+/3}\left(\frac{m}{u}\right)^2\frac{\sqrt{\pi}\Gamma\left(1-\frac{2K_+}{3}\right)^3}{4\Gamma\left(\frac{3}{2}-\frac{2K_+}{3}\right)}{}_3F_2\left(1-\frac{2K_+}{3},1-\frac{2K_+}{3},1-\frac{2K_+}{3};\frac{3}{2}-\frac{2K_+}{3},1;-\frac{\omega^2+(uq)^2}{4m^2}\right), \tag{55}$$

where $\Gamma(x)$ is the gamma function and ${}_3F_2(\ldots;\ldots;z)$ is a generalized hypergeometric function [132]. Compared with Eq. (55), the imaginary part of the exact response function would possess thresholds at frequency integer multiples of $2m$ associated with the excitation of more than one pair of kinks in the intermediate state. However, expression (55) is *exact* as long as $\omega<4m$. For the fermions, the expression of the structure factor is exact and reads

$$\chi^F_{\rho\rho}(\pm 2k_F+q,\omega)=\frac{1}{2\pi u}\left(\frac{m\alpha}{u}\right)^{K_+/3}\left[\frac{\Gamma\left(1-\frac{K_+}{6}\right)^3}{\Gamma\left(\frac{3}{2}-\frac{K_+}{6}\right)}{}_3F_2\left(1-\frac{K_+}{6},1-\frac{K_+}{6},1-\frac{K_+}{6};\frac{3}{2}-\frac{K_+}{6},1;-\frac{\omega^2+(uq)^2}{4m^2}\right)\right.$$
$$\left.+\frac{\Gamma\left(2-\frac{K_+}{6}\right)\Gamma\left(1-\frac{K_+}{6}\right)\Gamma\left(-\frac{K_+}{6}\right)}{\Gamma\left(\frac{3}{2}-\frac{K_+}{6}\right)}{}_3F_2\left(2-\frac{K_+}{6},1-\frac{K_+}{6},-\frac{K_+}{6};\frac{3}{2}-\frac{K_+}{6},1;-\frac{\omega^2+(uq)^2}{4m^2}\right)\right]. \tag{56}$$

Since the generalized hypergeometric functions ${}_{p+1}F_p(\ldots;\ldots;z)$ are analytic for $|z|<1$ [133], the imaginary part of the response functions is vanishing for $\omega<2m$. For $\omega>2m$, the behavior of the imaginary part above the threshold is obtained from a theorem quoted in Ref. [134]. One finds for $\omega\lesssim 2m$:

$$\mathrm{Im}\,\chi^F_{\rho\rho}(\pm 2k_F+q,\omega)\sim(\omega^2-(uq)^2-(2m)^2)^{K_+/3-1/2}, \tag{57}$$

for the unpaired atoms, and

$$\mathrm{Im}\,\chi^B_{\rho\rho}(\pm 2k_B+q,\omega)\sim(\omega^2-(uq)^2-(2m)^2)^{4K_+/3-1/2} \tag{58}$$

in the case of the molecules. Therefore, for sufficiently strong repulsion, the imaginary parts of both density-density response functions have a power law divergence for $\omega\to 2m+0$. For weaker repulsion, $3/8<K_+<9/8$, the divergence in the molecule density-density response is replaced by a cusp which disappears if $K_+>9/8$. Similarly, for $3/2<K_+<9/2$ the divergence in the unpaired atoms density density correlator is replaced by a cusp, which disappears if $K_+>9/2$. The imaginary parts of correlation functions Eqs. (55) and (56) can be measured by Bragg spectroscopy [135–137]. In Fig. 5 we plot the imaginary part of density correlation functions for the molecules with $K_+=1/4$ (in which case we have a divergence at the threshold) and $K_+=1/2$ (in which case there is only a cusp at threshold) as a function of frequency.

3. Spectral functions of the fermions

At the Luther-Emery point, it is also possible to calculate the spectral functions of the original fermions $\psi_{r,\sigma}$ (not the

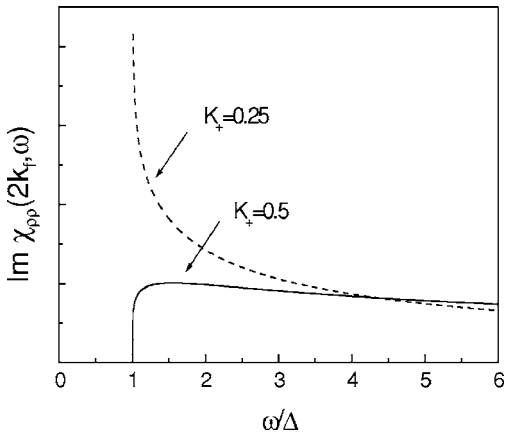

FIG. 5. The imaginary part of the density-density correlation function for the bosonic system with $K_+=1/4,1/2$.

pseudofermions $\Psi_{r,\sigma}$). To obtain these spectral functions, we express the operators $\psi_{r,\sigma}$ as a function of the fields $\phi_+,\Phi_{\uparrow,\downarrow}$ and their dual fields as

$$\psi_{+,\sigma}(x)=\frac{1}{\sqrt{2\pi\alpha}}e^{(i/\sqrt{6})(\theta_+-\phi_+)}e^{i[-\Theta_{-\sigma}+(5/6)\Phi_{-\sigma}]}e^{-(i/6)\Phi_\sigma}, \tag{59}$$

$$\psi_{-,\sigma}(x)=\frac{1}{\sqrt{2\pi\alpha}}e^{(i/\sqrt{6})(\theta_++\phi_+)}e^{i[\Theta_\sigma+(5/6)\Phi_\sigma]}e^{-(i/6)\Phi_{-\sigma}}. \tag{60}$$

Therefore, the Green's function of the fermionic atoms factorizes as

$$-\langle T_\tau\psi_{+,\sigma}(x,\tau)\psi_{+,\sigma}(0,0)\rangle=G_+(x,\tau)G_{-\sigma}^{-1,5/6}(x,\tau)G_\sigma^{0,1/6}(x,\tau). \tag{61}$$

The Green's function G_+ can be calculated by the standard methods of bosonization [54]. Since the fields Φ_σ are long-range ordered, the correlator $G_\sigma^{0,1/6}$ contributes a constant prefactor.

Therefore, we are left with $G_{-\sigma}^{-1,5/6}$ to evaluate. This is done following the method of Refs. [138–140]. In final form, the Fourier transform of the Fermion Green's function reads

$$\hat{G}(q,\omega_n)\sim {}_2F_1\left(\frac{7}{4}-\frac{1}{24}(K_++K_+^{-1}),\frac{13}{12}-\frac{1}{24}(K_++K_+^{-1});2;-\frac{(uq)^2+\omega_n^2}{m^2}\right). \tag{62}$$

When this Green's function is analytically continued to real frequency, it is seen [129] that it has a power law singularity for $\omega^2=(uq)^2+m^2$, and is analytic for ω below this threshold. As a result, the fermion Green's function vanishes below the gap, as it would do in a superconductor [141]. However the anomalous Green's function is still vanishing [142], in accordance with the theorem of Mermin-Wagner-Hohenberg [69,70].

IV. MOTT INSULATING STATE

Until now, we have only considered the case of the continuum system (1) or incommensurate filling in the lattice system (2). We now turn to a lattice system at commensurate filling. We first establish a generalization of the Lieb-Schultz-Mattis theorem [143–148] in the case of the boson-fermion mixture described by the Hamiltonian (2). This will give us a condition for the existence of a Mott insulating state without spontaneous breakdown of translational invariance. Then, we will discuss using bosonization the properties of the Mott state. We note that Mott states have been studied in the boson-fermion model in Refs. [81,106], but not in a one-dimensional case. Finally, we will consider the case when the molecules or the atoms can form a Mott insulating case in the absence of boson-fermion conversion, and we will show that this Mott state is unstable.

A. Generalized Lieb-Schultz-Mattis theorem

A generalized Lieb-Schultz-Mattis theorem can be proven for the boson fermion mixture described by the lattice Hamiltonian (2) [143,144,146,147]. Let us introduce the operator:

$$U=\exp\left[i\frac{2\pi}{N}\sum_{j=1}^{N}(2b_j^\dagger b_j+f_{j,\downarrow}^\dagger f_{j,\downarrow}+f_{j,\uparrow}^\dagger f_{j,\uparrow})\right], \tag{63}$$

such that $U^\dagger H_{bf}U=H_{bf}$. Following the arguments in Ref. [147], one has

$$\langle 0|U^\dagger HU-H|0\rangle=O\left(\frac{1}{N}\right), \tag{64}$$

$$U^\dagger TU=Te^{i2\pi\nu}, \tag{65}$$

where $|0\rangle$ is the ground state of the system, T is the translation operator, and H is the full Hamiltonian. The quantity ν is defined by

$$\nu=\frac{1}{N}\sum_{j=1}^{N}\left(2b_j^\dagger b_j+\sum_\sigma f_{j,\sigma}^\dagger f_{j,\sigma}\right)=\frac{1}{N}(2N_b+N_f). \tag{66}$$

For noninteger ν, it results from the analysis of [147] that there is a state $U|0\rangle$ of momentum $2\pi\nu\neq 0[2\pi]$ which is orthogonal to the ground state $|0\rangle$ and is only $O(1/N)$ above the ground state. This implies either a ground state degeneracy (associated with a spontaneous breaking of translational symmetry) or the existence of gapless excitations (if the spontaneous translational symmetry is unbroken and the ground state is unique). For integer ν, the ground state and the state $U|0\rangle$ have the same momentum. In that case, a gapped state without degeneracy can be obtained. This state is analogous to the Mott insulating state in the half-filled Hubbard model in one dimension [149] or the Mott insulating state in the Bose-Hubbard model with one boson per site [94]. We note that for $\lambda=0$ in the Hamiltonian (2) fermions and bosons are separately conserved, and the respective Fermi and pseudo-Fermi wave vectors are: $k_F=\pi N_F/2N$ and $k_B=\pi N_B/N$. The momentum of the state $U|0\rangle$ is thus equal to

$4(k_B+k_F)$. The condition to have a Mott insulating state in the Hubbard model, $4k_F=2\pi$ is thus generalized in the boson-fermion model to $4(k_B+k_F)=2\pi$, i.e., $2N_b+N_f=N$.

B. Umklapp term

In this section, we provide a derivation of the umklapp term valid in the case of the lattice system (2). Let us consider the $2k_F$ and $2k_B$ components of the atom and molecule charge density, given, respectively, by Eqs. (18) and (19). These terms yield an interaction of the form:

$$\frac{C}{2}\int \cos[2\phi_b+\sqrt{2}\phi_\rho-2(k_B+k_F)x]\cos\sqrt{2}\phi_\sigma + \frac{C}{2}\int \cos[2\phi_b-\sqrt{2}\phi_\rho-2(k_B-k_F)x]\cos\sqrt{2}\phi_\sigma. \tag{67}$$

In Eq. (67), the last line is the backscattering term of Eq. (22), and the second line is the umklapp term. Let us consider a case with $k_F\neq k_B$, and let us concentrate on the effect of the umklapp term. Using the rotation (25), we can reexpress it as

$$\frac{C}{2}\int dx\cos[\sqrt{6}\phi_+-2(k_B+k_F)x]\cos\sqrt{2}\phi_\sigma. \tag{68}$$

In the following we will consider the cases corresponding to one or two atoms per site.

1. Mott insulating state with one atom per site

Let us consider first the case of $(k_B+k_F)=\pi/2\alpha$. Then, the term (68) is oscillating. In second-order perturbation theory, it gives rise to the umklapp term:

$$H^{1F}_{\text{umk.}}=\frac{2g_U}{(2\pi\alpha)^2}\int dx\cos\sqrt{24}\phi_+. \tag{69}$$

The condition for the appearance of the umklapp term (69) can be seen to correspond to having one fermion atom per site of the atomic lattice. Let us briefly mention two alternative derivations of Eq. (69). A first derivation is obtained by considering the combination of the $4k_B$ term in the boson density with the $4k_F$ term in the fermion density in Haldane's expansion [60]. A second derivation is obtained by considering the effect of a translation by one lattice parameter on the phases ϕ_ρ and ϕ_b [147,150]. The expressions of the densities (18) and (19) imply that upon a translation by a single site $\phi_\rho\rightarrow\phi_\rho-\sqrt{2}k_F\alpha$ and $\phi_b\rightarrow\phi_b-k_B\alpha$. Therefore, the combination $\sqrt{6}\phi_+=2\phi_b+\sqrt{2}\phi_\rho$ transforms as: $\sqrt{6}\phi_\pm\rightarrow\sqrt{6}\phi_+-2(k_B+k_F)\alpha$. For $2(k_F+k_B)=\pi/\alpha$, the term $\cos 2\sqrt{6}\phi_+$ is invariant upon translation, thus leading again to Eq. (69). The presence of the umklapp term (69) in the Hamiltonian can result in the opening of a charge gap and the formation of a Mott insulating state provided the operator $\cos\sqrt{24}\phi_+$ is relevant. Since the umklapp term is of dimension $6K_+$ this implies that a Mott insulating state is possible only for $K_+<1/3$, i.e., very strong repulsion. By comparison, in the case of fermions, the Mott transition would occur at $K_\rho=1$, i.e., for weakly repulsive interaction [54]. Thus, the Josephson coupling (23) is very effective in destabilizing the Mott state. In the Mott insulating state, the superfluid fluctuations become short ranged. Since CDW fluctuations are also suppressed, the system shows some analogy with the Haldane gapped phase of spin-1 chains [151] in that it is totally quantum disordered. In fact, this analogy can be strengthened by exhibiting an analog of the VBS (valence bond solid) order parameter [152,153]. In Haldane gapped chains, this nonlocal order parameter measures a hidden long-range order in the system associated with the breakdown of a hidden discrete symmetry in the system. The equivalent nonlocal order parameter for the atom-molecule system is discussed in Appendix C.

2. Mott insulating state with two atoms per site

Another commensurate filling, where a Mott insulating state is possible is obtained for $(k_F+k_B)=\pi/\alpha$. This case corresponds to having one molecule (or two atoms) per site of the optical lattice. In that case, the term in Eq. (68) is nonoscillating, and it gives rise to an umklapp term of the form:

$$H^{1B}_{\text{umk}}=\frac{2g_U}{(2\pi\alpha)^2}\int dx\cos\sqrt{6}\phi_+\cos\sqrt{2}\phi_\sigma. \tag{70}$$

We notice that this umklapp term is compatible with the spin gap induced by the Josephson term (23). When the Josephson coupling is large, we can make $\cos\sqrt{2}\phi_\sigma\rightarrow\langle\cos\sqrt{2}\phi_\sigma\rangle$ and we see that the term (70) becomes relevant for $K_+=4/3$. For weaker Josephson coupling, the dimension becomes $1/2+3/2K_+$, and this term is relevant only for $K_+<1$. Since $K_+=1$ corresponds to hard core bosons, this means that for weak Josephson coupling, the Mott state with a single boson per site becomes trivial. Interestingly, we note that increasing the Josephson coupling is *enhancing* the tendency of the system to enter a Mott insulating state as a result of the formation of a spin gap. If we compare with a system of bosons at commensurate filling, we note however that the Mott transition would obtain for $K_b=2$ [54]. Therefore, the Josephson coupling still appears to weaken the tendency to form a Mott insulating state. Such tendency was also observed in Ref. [81].

C. Commensurate filling of the atomic or molecular subsystem

When the atomic subsystem is at commensurate filling $(4k_F=2\pi/a)$, an umklapp term:

$$\frac{-2g_3}{(2\pi\alpha)^2}\cos\sqrt{8}\phi_\rho, \tag{71}$$

must be added to the Hamiltonian. Such umklapp term can create a gap in the density excitations of the unpaired atoms. However, we must also take into account the term (23). This term is ordering θ_- and thus competes with the umklapp term (71). To understand what happens when θ_- is locked, it is convenient to rewrite the umklapp term (71) as $\propto\cos\sqrt{8/3}(\sqrt{2}\phi_+-\phi_-)$. The terms generated by the renormalization group are of the form $\cos n\sqrt{8/3}(\sqrt{2}\phi_+-\phi_-)$, with n an integer. When θ_- is locked, replacing the terms $e^{i\beta\phi_-}$ by

their expectation values, we find that all these terms vanish. Therefore, no term $\cos\beta\phi_+$ can appear in the low energy Hamiltonian. A more formal justification of the absence of the $\cos\beta\phi_+$ term in the low energy Hamiltonian can be given by noting that when the Hamiltonian is expressed in terms of $\phi_\pm$ it has a continuous symmetry $\phi_+\to\phi_++\alpha$ and $\phi_-\to\phi_-+\sqrt{2}\alpha$. As a result, terms of the form $\cos\beta\phi_+$ are forbidden by such symmetry. The consequence of the absence of $\cos\beta\phi_+$ terms in the Hamiltonian when θ_- is locked is that, even if the unpaired atom density is at a commensurate filling, the umklapp terms do not destabilize the coupled phase. However, in the opposite case of a strong umklapp term and a weak boson-fermion conversion term, it is the field ϕ_ρ that will be ordered. The previous arguments can be reversed and show that the formation of a Mott gap for the fermions will prevent the formation of the coupled phase. Using the method of Ref. [154], one can show that the phase transition between the coupled and the decoupled state is identical to the phase transition that occurs in two nonequivalent coupled two-dimensional *XY* models. This phase transition was studied by the renormalization group in Refs. [155,156]. It was found that in the case of interest to us, this phase transition was in the Ising universality class. Thus, one expects a quantum Ising phase transition between the state where the fermions are decoupled from the bosons and form a Mott insulator and the state where the fermions and bosons are coupled and form a superfluid.

Of course, the same arguments can also be applied to the bosons at commensurate filling, the role of the fields ϕ_b and ϕ_ρ being simply reversed.

V. RELATION WITH EXPERIMENTS

A. Without a potential along the tubes

To connect experiments in quasi-one-dimensional confining waveguides with theoretical models in 1D, it is necessary to obtain estimates of the parameters that enter the Hamiltonians (2) and (1) and the bosonized Hamiltonian (13), (23), and (20). Since the parameters in the Hamiltonian (2) depend on the periodic optical trapping potential, we will mainly focus on the parameters that enter in the continuum Hamiltonian Eq. (1) and in the bosonized Hamiltonian, i.e., the Luttinger exponent K_ρ, the velocity, and the fermion-boson coupling λ. Before giving an estimate of the parameters we need first to recall that, at the two-body level, there is a connection between the 1D boson-fermion model and the quasi-1D single channel model [76], thus we will use one or the other depending on the physical parameter wherein we are interested. Experimentally, molecules have been formed from fermionic atoms ^{6}Li [12,14,15,21] and ^{40}K [13,20,67]. For ^{6}Li, the mass of an atom is $m_F(^6\mathrm{Li})=9.6\times10^{-27}$ kg, and for ^{40}K it is $m_F(^{40}K)=6.4\times10^{-26}$ kg. In ^{6}Li, a narrow Feshbach resonance was obtained in a magnetic field of $B=543$ G, with a width $\Delta B=0.23$ G [14,157]. In the following, we will focus on this resonance.

Before discussing the microscopic interactions, let us determine the real space cutoff α in Eqs. (22) and (23). Since as long as the kinetic energy of longitudinal motion of the particles is much smaller than the trapping energy $\hbar\omega_\perp$, the system behaves as a one-dimensional one, bosonization is applicable for length scales ℓ such that $\hbar v_F/\ell\ll\hbar\omega_\perp$ [158]. The real space cutoff is thus $\alpha\sim v_F/\omega_\perp$. Having found the real space cutoff, we turn to the interaction parameters. The interaction in an atomic gas is measured by a parameter $g_{3D}=4\pi\hbar^2a_s/m$, a_s being the atom-atom scattering length. In the case of ^{6}Li, $a_s=45a_0$ where $a_0\sim5\times10^{-11}$ m is the Bohr radius [159–162]. The effective one-dimensional interaction has been derived in Refs. [66,163]. We can estimate the effective interaction strength from Eq. (43) in Ref. [66] to be: $g_{1D}=(4\hbar a_s/ma_\perp^2)(1-Ca_s/a_\perp)$, where $C\simeq1.46$. The confinement induced resonance results in an enhancement of the one-dimensional effective interaction by a factor $(1-Ca_s/a_\perp)^{-1}$. Using the measured scattering length, and estimating $a_\perp$ from the harmonic oscillator formula with $\omega_\perp\sim2\pi\times100$ kHz, we find that the enhancement factor is of order 1.04. Thus, CIR is not affecting strongly the effective one dimensional interaction strength. We now turn to the boson-fermion conversion factor. In the three-dimensional case [7,164], it is given by

$$\lambda_{3D}=\hbar\sqrt{\frac{4\pi a_s\Delta\mu\Delta B}{m}}, \tag{72}$$

where a_{bg} is the atom-atom scattering length far from resonance, ΔB is the width of the resonance, and $\Delta\mu$ is the difference of magnetic moment between atom and molecule. In Ref. [165], it was shown that in the case of a narrow resonance, there is no renormalization of $\Delta\mu$, so that $\Delta\mu=1$ in the case of ^{6}Li. According to Eq. (44) in Ref. [66], we have $\lambda_{1D}^2=(2a_s\mu\Delta/ma_\perp^2)(1-Ca_s/a_\perp)^{-2}$. Again, the enhancement coming from the CIR is of order 1.

The condition for perturbation theory to be valid is that the energy associated with the formation of molecules, $\lambda_{1D}\alpha^{-1/2}$ is small with respect to the energy cutoff $\hbar\omega_\perp$. Therefore, perturbation theory is applicable when: $\lambda/\hbar(v_F\omega_\perp)^{1/2}\ll1$, i.e.,

$$\frac{a_s\mu\Delta B}{\hbar v_F}\ll1. \tag{73}$$

Using the values given in Refs. [14,165], we find that this ratio is small for $v_F\gg3.2\times10^{-2}$ m/s. Since v_F can be expected to be of the order of 10^{-3} m/s, this is not unreasonable. In fact, using the values of the trapping frequency given by Moritz *et al.* [67] we find that: $v_F=4.6\times10^{-2}$ m/s so that in ^{6}Li at the narrow resonance, the ratio is of order 0.7 and we can expect our theory to be qualitatively valid.

Concerning K_ρ, we find using Eq. (43) in Ref. [66] and the perturbative expression of the Luttinger exponent [54] that: $K_\rho\simeq0.995$, i.e., interactions between fermions can be neglected. Since the interaction between the molecules [166] has a scattering length $a_{BB}=0.6a_{FF}$ one sees that molecules also are only weakly interacting. As a result, one expects that without a potential along the tubes, only the phase with coherence between atoms and molecules can be observed.

B. With a potential along the tubes

As we have seen in Sec. V A, in the case of a two-dimensional optical lattice without periodic potential along

the tubes, the repulsion between the bosonic molecules is weak, making the decoupling transition or the Mott transition impossible to observe. To increase the effect of the repulsion, one needs to increase the effective mass of the atoms by adding a periodic potential along the tubes. In fact, it has been shown in the case of bosonic ^{87}Rb atoms that this enhancement could be strong enough to push the system in the Tonks-Girardeau regime [50]. A periodic potential can be imposed along the tubes by placing the atoms in a three-dimensional optical lattice. The atoms experience a potential:

$$V(x,y,z) = V_x \sin^2\left(\frac{2\pi x}{\lambda_l}\right) + V_y \sin^2\left(\frac{2\pi y}{\lambda_l}\right) + V_z \sin^2\left(\frac{2\pi z}{\lambda_l}\right), \tag{74}$$

where λ_l is the wavelength of the laser radiation, and $V_x \ll V_y, V_z$ so that the system remains quasi one-dimensional. The strength of the potential is measured in unit of the recoil energy $E_R=(\hbar^2/2m)\left(\frac{2\pi}{\lambda_l}\right)^2$ as $V_x=sE_R$. Typical values for s are in the range 5 to 25. For lithium atoms [167], the typical value of E_R is 76 kHz. If the potential is sufficiently strong, the atoms tend to localize in the lowest trap states near the minima of this potential. In our case, since the periodic potential along the tubes has shallower minima than in the transverse directions, the small overlap between the trap states in the longitudinal direction yields the single band Hamiltonian (2) [85,86]. An expression of the parameters of the lattice model (2) in terms of the microscopic parameters has been derived in Ref. [86]. On the lattice, the Fermi velocity of the atoms and the pseudo-Fermi velocity of the molecules can be reduced by increasing the depth of the periodic potential in the longitudinal direction. This allows one, in principle, to move the system near the decoupling transition [78] or the Mott transition, by reducing K_ρ.

A second possible setup [168] is to use a cigar shaped potential:

$$V_{\text{cigar}}(x,y,z) = \tfrac{1}{2} m\omega_0^2 (x^2 + \mu^2 \mathbf{r}_\perp^2), \tag{75}$$

with $\mu \gg 1$, so that the atoms and the molecules are strongly confined in the transverse direction, and to apply a periodic potential:

$$V_{\text{periodic}} = V_0 \sin^2\left(\frac{\pi x}{d}\right), \tag{76}$$

in order to form the one-dimensional structure described by the model (2).

The main difficulty of experiments in optical lattices is that the reduction of the bandwidth results in a reduction of the Fermi velocity v_F. Since the perturbative regime is defined by $\lambda\alpha^{1/2} \ll v_F$, this implies that by increasing the depth of the potential in the longitudinal direction one is also pushing the system in the regime where the boson-fermion conversion term must be treated nonperturbatively [76]. However, in that regime there is no longer coexistence of atoms and molecules and the decoupling transition does not exist. Moreover, in that regime, the Mott transition becomes the usual purely fermionic or purely bosonic Mott transition [54].

VI. CONCLUSIONS

We have studied a one-dimensional version of the boson-fermion model using the bosonization technique. We have found that at low energy the system is described by two Josephson coupled Luttinger liquids corresponding to the paired atomic and molecular superfluids. Due to the relevance of the Josephson coupling for not too strong repulsion, the order parameters for the Bose condensation and fermion superfluidity become identical, while a spin gap and a gap against the formation of phase slips are formed. As a result of these gaps, we have found that the charge density wave correlations decay exponentially, differently from the phases where only bosons or only fermions are present [75,76]. We have discussed the application of a magnetic field that results in a loss of coherence between the bosons and the fermion and the disappearance of the gap, while changing the detuning has no effect on the existence of the gaps until either the fermion or the boson density is reduced to zero. We have discussed the effect of a backscattering term which induces mutual locking of the density of bosons and fermions favoring charge density wave fluctuations resulting in a quantum Ising phase transition between the density wave phase and the superfluid phase. We have found a Luther-Emery point where the phase slips and the spin excitations can be described in terms of pseudofermions. For this special point in the parameter space, we have derived closed form expressions of the density-density correlations and the spectral functions. The spectral functions of the fermions are gapped, whereas the spectral functions of the bosons remain gapless but with an enhanced divergence for momentum close to zero. Finally, we have discussed the formation of a Mott insulating state in a periodic potential at commensurate filling. We have first established a generalization of the Lieb-Schulz-Mattis theorem, giving the condition for the existence of a Mott-insulating state without spontaneous breakdown of translational invariance. Then, we have discussed the properties of the Mott state in the case of one atom or two atoms per site showing that in the first case the Josephson coupling is very effective in destabilizing the Mott state. Finally, we have considered the case when the atoms or the molecules can form a Mott state in absence of boson-fermion conversion and shown that this Mott state is unstable. To connect our results with experiments in quasi-one-dimensional confining waveguides we have derived estimates of the parameters that enter the bosonized Hamiltonian, as the Luttinger exponents, using the values of the trapping frequency and density used in experiments. We have seen that bosons are only weakly interacting and the necessary small fermionic Luttinger parameter required us to realize a strongly interacting system, rendering the Mott insulating and decoupled phases difficult to observe in experiments. A nontrivial challenge is the experimental realization of the coupled Luttinger liquids phase with parameters tunable through the exactly solvable point (the Luther-Emery point). We suggest that a Fano-Feshbach resonantly interacting atomic gas confined in a highly anisotropic (1d) trap and subject to a periodic optical potential is a promising candidate for an experimental measurement of the physical quantities (correlation functions) discussed here. Finally we would like to comment on

the fact that an interesting edge states physics is expected when open boundary conditions (or a cut one-dimensional boson-fermion system) are considered. The existence of edge states at the end of the system could lead to significant contribution to the density profile that could be tested in experiments. The physics of the edge states will be similar to the one of Haldane gap systems, like the valence bond solid model, and a study along this direction is in progress.

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APPENDIX A: EXPRESSION OF THE LUTTINGER PARAMETERS OF THE ROTATED HAMILTONIAN

The Luttinger parameters of the rotated Hamiltonian (26) can be straightforwardly obtained in the form:

$$u_+K_+ = \tfrac{2}{3}u_bK_b + \tfrac{1}{3}u_\rho K_\rho,$$

$$u_-K_- = \tfrac{1}{3}u_bK_b + \tfrac{2}{3}u_\rho K_\rho,$$

$$g_1 = \frac{\sqrt{8}}{3}(u_bK_b - u_\rho K_\rho),$$

$$\frac{u_+}{K_+} = \frac{2u_b}{3K_b} + \frac{u_\rho}{3K_\rho} + \frac{4V}{3\pi}, \tag{A1}$$

$$\frac{u_-}{K_-} = \frac{u_b}{3K_b} + \frac{2u_\rho}{3K_\rho} - \frac{4V}{3\pi}, \tag{A2}$$

$$g_2 = \frac{\sqrt{8}}{3}\left(\frac{u_b}{K_b} - u_\rho K_\rho - \frac{V}{\pi}\right), \tag{A3}$$

by substituting the expressions of Π_b, ϕ_b and Π_ρ, ϕ_ρ in terms of the new fields $\Pi_\pm, \phi_\pm$ in the original quadratic Hamiltonian.

APPENDIX B: CALCULATION OF THE INTEGRALS IN EQS. (55) AND (56)

In this appendix we will derive a slightly more general integral than those of Eqs. (55) and (56). Namely, we will consider

$$g(y) = \int_0^\infty K_\mu(u)K_\nu(u)J_\lambda(yu)u^\alpha du. \tag{B1}$$

To find Eq. (B1) explicitly, we use the series expansion of the Bessel function J_λ from Ref. [129] [Eq. (9.1.10)]. We find that

$$g(y) = \left(\frac{y}{2}\right)^\lambda \sum_{k=0}^\infty \left(-\frac{y^2}{4}\right)^k \frac{1}{\Gamma(k+1)\Gamma(k+\lambda+1)} \times \int_0^\infty K_\mu(u)K_\nu(u)u^{2k+\lambda+\alpha}du. \tag{B2}$$

The integral that appears in the expansion in powers of y^2 is a well-known Weber-Schaefheitlin integral [169] with two modified Bessel functions. Its expression is

$$\int_0^\infty K_\mu(u)K_\nu(u)u^{2k+\alpha+\lambda}du = \frac{2^{2(k-1)+\alpha+\lambda}}{\Gamma(2k+\alpha+\lambda+1)}\Gamma\left(k+\frac{1+\nu+\mu+\alpha+\lambda}{2}\right)\Gamma\left(k+\frac{1+\nu-\mu+\alpha+\lambda}{2}\right) \times\Gamma\left(k+\frac{1-\nu+\mu+\alpha+\lambda}{2}\right)\Gamma\left(k+\frac{1-\nu-\mu+\alpha+\lambda}{2}\right), \tag{B3}$$

The resulting expression of $g(y)$ can be rearranged using the duplication formula for the Gamma function, Eq. (6.1.18) in Ref. [129]. The final expression of g is

$$g(y) = \left(\frac{y}{2}\right)^\lambda \frac{\pi^{1/2}}{4} \times\sum_{k=0}^\infty \frac{\Gamma\left(k+\frac{1+\nu+\mu+\alpha+\lambda}{2}\right)\Gamma\left(k+\frac{1+\nu-\mu+\alpha+\lambda}{2}\right)\times\Gamma\left(k+\frac{1-\nu+\mu+\alpha+\lambda}{2}\right)\Gamma\left(k+\frac{1-\nu-\mu+\alpha+\lambda}{2}\right)}{\Gamma\left(k+1+\frac{\alpha+\lambda}{2}\right)\Gamma\left(k+\frac{\alpha+\lambda+1}{2}\right)\Gamma(k+\lambda+1)} \times\frac{1}{k!}\left(-\frac{y^2}{4}\right)^k. \tag{B4}$$

This series expansion is readily identified with the definition of the generalized hypergeometric function ${}_4F_3$ given in [133]. So we find finally that

$$g(y)=\frac{\sqrt{\pi}}{4}\left(\frac{y}{2}\right)^{\lambda}\frac{\Gamma\left(\frac{1+\nu+\mu+\alpha+\lambda}{2}\right)\Gamma\left(\frac{1+\nu-\mu+\alpha+\lambda}{2}\right)\Gamma\left(\frac{1-\nu+\mu+\alpha+\lambda}{2}\right)\Gamma\left(\frac{1-\nu-\mu+\alpha+\lambda}{2}\right)}{\Gamma\left(1+\frac{\alpha+\lambda}{2}\right)\Gamma\left(\frac{\alpha+\lambda+1}{2}\right)\Gamma(\lambda+1)}$$

$$\times {}_4F_3\left(\frac{1+\alpha+\lambda+\nu+\mu}{2},\frac{1+\alpha+\lambda+\nu-\mu}{2},\frac{1+\alpha+\lambda-\nu+\mu}{2},\frac{1+\alpha+\lambda-\nu-\mu}{2};1+\frac{\alpha+\lambda}{2},\frac{\alpha+\lambda+1}{2},1+\lambda;-\frac{y^2}{4}\right). \tag{B5}$$

For $\nu=\mu$, the function ${}_4F_3$ reduces to a simpler ${}_3F_2$ function. This leads to Eqs. (55) and (56).

APPENDIX C: NONLOCAL ORDER PARAMETER FOR THE MOTT STATE

The Mott insulating state can be characterized by the expectation value of a nonlocal order parameter as the Haldane gap state in a spin-1 chain [153,152]. The nonlocal order parameter is defined as follows:

$$O(k,l)=\left\langle b_k^\dagger b_k\prod_{j>k}^{l}e^{-i(2\pi/3)(2b_j^\dagger b_j+\Sigma_\sigma f_{j,\sigma}^\dagger f_{j,\sigma})}b_l^\dagger b_l\right\rangle \tag{C1}$$

The string operator:

$$O_{\text{string}}(k,l)=\prod_{j>k}^{l}e^{-i(2\pi/3)(2b_j^\dagger b_j+\Sigma_\sigma f_{j,\sigma}^\dagger f_{j,\sigma})} \tag{C2}$$

is a product of exponentials. As a result of its definition, we see that it is counting the number of fermions located between the sites k and l, either unbound or forming a molecule. To derive a bosonized expression of this operator, we notice that $\exp(2i\pi b_j^\dagger b_j)=1$ since $b_j^\dagger b_j$ has only integer eigenvalues and rewrite the string operator as

$$\prod_{j>k}^{l}e^{i(2\pi/3)(b_j^\dagger b_j-\Sigma_\sigma f_{j,\sigma}^\dagger f_{j,\sigma})}. \tag{C3}$$

Using bosonization and Eq. (C2), we find

$$O_{\text{string}}(x,x')=\exp\left[i\frac{2\pi}{3}(\rho_B-\rho_F)(x-x')-\frac{2}{\sqrt{3}}(\phi_-(x)-\phi_-(x'))\right]. \tag{C4}$$

Using Eqs. (40) and (C4) we obtain the nonlocal order parameter (C1) as

$$O(x,x')=\langle e^{i\sqrt{(8/3)}(\phi_+(x)-\phi_+(x'))-i2\pi/3(2\rho_B+\rho_F)(x-x')}\rangle. \tag{C5}$$

In the Mott insulating state with one fermion per site, we have $4(k_F+k_B)=2\pi(2\rho_B+\rho_F)=2n\pi$ where n is an integer. Taking $x,x'\to\infty$, we see that the expectation value of the order parameter is nonvanishing in the Mott state.

A related VBS type order parameter can be defined as

$$O'(k,l)=\left\langle\left(\sum_\sigma f_{k,\sigma}^\dagger f_{k,\sigma}\right)\prod_{j>k}^{l}e^{i(2\pi/3)(b_j^\dagger b_j-\Sigma_\sigma f_{j,\sigma}^\dagger f_{j,\sigma})}\times\left(\sum_\sigma f_{l,\sigma}^\dagger f_{l,\sigma}\right)\right\rangle \tag{C6}$$

In bosonized form, we have

$$O'(x,x')=\langle e^{i\sqrt{(4/3)}(\phi_+(x)-\phi_+(x'))+i\pi/3(2\rho_B+\rho_F)(x-x')}\rangle, \tag{C7}$$

and again this order parameter is nonvanishing. The physical interpretation of the nonzero expectation value of these nonlocal order parameters is that both bosons and fermions possess a hidden charge density wave order in the Mott insulator. This charge density wave is hidden as a result of the fluctuation of the density of fermions and the density of bosons.

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