

Excitations of one-dimensional supersolids with optical lattices

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Based on mean-field Gross-Pitaevskii and Bogoliubov–de Gennes approaches, we investigate excitations of a one-dimensional soft-core interacting ultracold Bose gas under the effect of an optical lattice. It is found that no matter how deep the lattice is, at $q \rightarrow 0$ the lowest mode corresponds to a gapless phonon, $\omega_1^2 = v_1^2 q^2$, whereas the second lowest mode corresponds to a gapped optical phonon, $\omega_2^2 = \Delta^2 \pm v_2^2 q^2$. Determination of the velocities v_1, v_2 , the gap Δ , and the possible sign change in ω_2 upon the change of lattice depth can give decisive measures to the transitions across various supersolid and solid states. The power law $v_1 \sim (f_s)^{1/2}$ with f_s the superfluid fraction is identified in the present system at the tight-binding regime.

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I. INTRODUCTION

Ultracold bosonic atoms with relatively short range or contact interaction in optical lattices can exhibit a superfluid (SF)–Mott insulator (MI) quantum phase transition by increasing the depth of the lattice potential [1,2]. In such a system, the lowest excitation at $\mathbf{q} \rightarrow 0$ may shift from a gapless phonon mode in the SF state to a gapped mode in the MI state [3]. On the other hand, ultracold atoms with sufficiently strong soft-core or laser-induced dipole-dipole interaction may exhibit a SF–supersolid (SS) transition in which crystalline and SF properties are simultaneously possessed in the SS state [4–10]. Excitations of such a system can change from having one gapless mode in the SF state to two gapless modes in the SS state for a given propagation direction [11–13]. The additional gapless (phonon) mode in the SS state manifests the breaking of the translational symmetry associated with the formation of the crystalline structure. Supersolidity was first predicted and discussed in the context of solid He⁴ by Andreev and Lifshitz [14], Chester [15], and Leggett [16].

Recently Macrì and Pohl [17] have proven the stability of a Rydberg-dressed atomic system—one of the leading candidates to display the supersolidity, confined in an optical lattice. More recently, Hsueh *et al.* [18] have shown that by loading the preformed Rydberg-dressed SS system into an optical lattice, upon increasing the depth of the lattice potential the system can undergo an *intrinsic-to-extrinsic* SS transition. In the intrinsic (or incommensurate) SS phase with relatively weaker lattice potential, atom droplets per lattice constant is a fraction ν [18] and the periodicity is governed by the effective range of the internal soft-core interaction. Whereas in the extrinsic (or commensurate) SS phase with relatively stronger lattice potential, the periodicity is governed by the lattice constant of the lattice potential. In addition, upon increasing the lattice depth, there could exist more than one incommensurate SS states before entering the commensurate SS state. It is worth noting that the case of loading preformed SS into an optical lattice is somewhat different from that of lattice supersolids [19–31].

This paper aims to study the excitations of a SS system under the effect of an optical lattice. In literature, based on a quantum Monte Carlo (QMC) calculation, Saccani *et al.* [11] have shown that for a given propagation direction the excitations of a supersolid without optical lattices can exhibit

an additional gapless mode in addition to the one responsible for the superfluid phase. Based on a Bogoliubov–de Gennes (BdG) approach, Macrì *et al.* [13] have further verified that in a SS system with two-dimensional hexagonal lattice, there are three gapless modes—one associated with the superfluid phase and two associated with the crystalline formation. Thus the change in the excitation spectrum from one to two gapless modes can be viewed as a general feature of the SF-SS transition if the crystal is robustly formed. Some exceptions include when there is an external potential that breaks the underlying lattice translation symmetry or when the system has an additional three-body interaction that results in the crystal being fragile. While Refs. [11–13] considered only the soft-core interacting systems, this feature should also hold for other long-range systems if the SF-SS transition is sustained [10]. A soft-core interaction potential with a finite flat range seems to be the most natural candidate for the SF-SS transition, however.

We will show that once lattice potential is in effect on the preformed SS, the lowest excitation mode remains gapless ($\omega_1^2 = v_1^2 q^2$) at $q \rightarrow 0$ when the system is first in an incommensurate SS state. However, for any propagation direction, the second lowest mode opens up a gap with the dispersion $\omega_2^2 = \Delta^2 + v_2^2 q^2$. When the lattice depth V_0 is increased such that the ground state changes from an incommensurate SS to a commensurate SS, a characteristic roton appears in the lowest gapless mode which is accompanied by a downward dispersion in the second lowest mode ($\omega_2^2 = \Delta^2 - v_2^2 q^2$). When lattice depth V_0 is further increased such that the system is away from the incommensurate-to-commensurate SS phase boundary, the roton disappears in the lowest mode and the second lowest mode turns upwards again ($\omega_2^2 = \Delta^2 + v_2^2 q^2$). Once lattice depth V_0 is greatly increased, phonon velocity v_1 of the lowest mode becomes vanishingly small, indicating that the system enters the solid state with the superfluid completely depleted, and a large gap Δ opens in the second lowest mode.

It has been deduced that in a superfluid with optical lattices, phonon velocity v_1 satisfies the following relationship $v_1^2 = 1/m^* \kappa$, with m^* the effective band mass and $\kappa = (n \partial \mu / \partial n)^{-1}$ the compressibility. (n is the mean atom density per lattice site and μ is the chemical potential [32,33].) In addition, superfluid fraction f_s of a lattice superfluid system was shown to be equal to m/m^* , with m the bare atom mass [34]. Thus, if

the compressibility κ remains constant upon the lattice depth change, there would be a power law between v_1^2 and f_s . This power law is indeed identified in the present soft-core system at the tight-binding regime.

II. FORMALISM

The following mean-field Gross-Pitaevskii energy functional of a one-dimensional (1D) soft-core interacting ultracold Bose gas in an optical lattice is considered:

$$E = \int \psi^*(x,t) \hat{h}_0 \psi(x,t) dx + \frac{1}{2} \int \int U(\bar{x}) |\psi(x',t)|^2 |\psi(x,t)|^2 dx' dx, \quad (1)$$

where $\hat{h}_0 = -\partial_x^2/2 + V_0 \sin^2(\pi x/d)$, with d the lattice constant and V_0 the depth of the lattice potential that corresponds to the single-particle part. Natural units $m = \hbar = 1$ are used. For the two-body interaction,

$$U(\bar{x}) = \gamma \delta(\bar{x}) + \alpha \theta(r_c - |\bar{x}|), \quad (2)$$

which can involve both contact and finite-range soft-core interactions ($\bar{x} \equiv x - x'$). For simplicity, a step-function-like soft-core interaction is employed with α and r_c , the strength and effective range (or blockade radius), respectively. This simplified interaction gives a good approximation for the effective soft-core interaction, $U(\bar{x}) \sim \alpha/[1 + (\bar{x}/r_c)^6]$, of the ultracold Rydberg-dressed Bose gas [35–38]. As we are focusing on the effect of the soft-core interaction, the contact interaction will be set to zero ($\gamma = 0$).

Elementary excitation out of a particular ground state can be studied via the Bogoliubov–de Gennes (BdG) equation. The fluctuations can be decomposed into different plane-wave modes labeled by q :

$$\delta\varphi_{k,q}(x,t) = u_{k,q} e^{iqx} e^{-i\omega_{k,q}t} + v_{k,q}^* e^{-iqx} e^{i\omega_{k,q}^*t}. \quad (3)$$

Consequently, the BdG equation of the present system is given by

$$\hat{\sigma}_3 M_{k,q} \begin{pmatrix} u_{k,q} \\ v_{k,q} \end{pmatrix} = \omega_{k,q} \begin{pmatrix} u_{k,q} \\ v_{k,q} \end{pmatrix}, \quad (4)$$

where $\hat{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and

$$M_{k,q} = \begin{bmatrix} \mathcal{L}_{q+k}(x) + U_k(x) & 0 \\ 0 & \mathcal{L}_{q-k}(x) + U_k(x) \end{bmatrix} + \begin{bmatrix} C_{k,q}(x)\varphi_k(x) & X_{k,q}(x)\varphi_k(x) \\ C_{k,q}(x)\varphi_k^*(x) & X_{k,q}(x)\varphi_k^*(x) \end{bmatrix} \quad (5)$$

is an $(8N + 2) \times (8N + 2)$ matrix, with N being the number of modes expanded in the corresponding ground-state wave function. Here $\mathcal{L}_{q \pm k}(x) \equiv (q \pm k)^2/2 + V_0 \sin^2(\pi x/d) - \mu_k$, $C_{k,q}(x) \equiv \bar{n}_0 \int U(\bar{x}) \varphi_k^*(x') e^{iq\bar{x}} dx'$, and $X_{k,q}(x) \equiv \bar{n}_0 \int U(\bar{x}) \varphi_k(x') e^{iq\bar{x}} dx'$, with \bar{n}_0 being the mean atom number per lattice constant.

III. GROUND STATES AND EXCITATIONS

Based on the Gross-Pitaevskii equation (GPE) and BdG formalism, we investigate the possible ground-state wave

functions and the corresponding excitation spectra of the system. By varying the lattice depth V_0 , Fig. 1 shows the ground-state density distributions vs space (top row) and in a reduced zone scheme the lowest two excitation spectra vs wave vector (bottom row) for representatives in various SS and solid states. All the lengths (energies) are in units of d (\hbar^2/md^2). In all cases, we have fixed $\bar{n}_0 \sim 10^3$, $\bar{n}_0\alpha \rightarrow \alpha = 30$, and $r_c = 4R^*/3$. R^* is defined such that when $r_c = R^*$, the intrinsic SS has spacing between neighboring droplets equal to d . In the current set of parameters, $R^* = 0.648d$. From the second left column to the right column correspond respectively to $\nu = 3/4$ incommensurate SS ($V_0 = 2.7$), $\nu = 4/5$ incommensurate SS ($V_0 = 11.7$), commensurate SS with $V_0 = 12$, commensurate SS with $V_0 = 30$, and the solid state ($V_0 = 192$). For comparison, the left column shows the cases for the intrinsic SS ($V_0 = 0$). ν is defined as the number of atom droplets per lattice constant. There exist two fractional ($\nu = 3/4$ and $\nu = 4/5$) incommensurate SS states in the present case.

As shown in the bottom row of Fig. 1, characteristics and dispersions of the lowest two excitation modes for various SS and solid states are summarized as follows. Two gapless modes occur for the intrinsic SS state, one associated with the superfluid phase and another associated with the formation of crystalline. When V_0 is finite but relatively weak such that the system is in the $\nu = 3/4$ incommensurate SS state, the lowest mode remains gapless ($\omega_1^2 = v_1^2 q^2$) at $q \rightarrow 0$ while the second lowest mode causes a small gap to open up with the dispersion $\omega_2^2 = \Delta^2 + v_2^2 q^2$ —signaling an out-of-phase density fluctuation for the current complex superfluid. When V_0 is increased with the system entering another ($\nu = 4/5$) incommensurate SS state, the main features of the lowest two modes are analogous to those for the $\nu = 3/4$ ones. When V_0 is further increased such that the ground state changes from an incommensurate SS to a commensurate SS ($\nu = 1$, atom peaks match lattice potential minima), a characteristic roton appears in the lowest mode which is accompanied by a downward dispersion in the second lowest mode ($\omega_2^2 = \Delta^2 - v_2^2 q^2$). The rotons, occurring at two wave vectors q_1 and q_2 , satisfy $q_1 + q_2 = 2\pi/d$. The onset of the roton signals the incommensurate-to-commensurate SS transition at $V_0 = V_c \simeq 11.9$ [18]. When V_0 is increased further such that the system is away from the incommensurate-to-commensurate SS phase boundary, the roton disappears in the lowest mode and the second lowest mode turns upwards again ($\omega_2^2 = \Delta^2 + v_2^2 q^2$). Once V_0 is greatly increased, phonon velocity v_1 of the lowest mode vanishes, indicating that the system is entering the solid state with superfluid completely depleted.

It is a general belief that mean-field treatment is applicable only when the order parameter is large and quantum fluctuation is small. In this regard, when the superfluid fraction is very small, the applicability of the mean-field GPE and BdG approaches could be questionable. At present, there is no justification on how good our results are when the superfluid fraction is very small. It will be seen when a non-mean-field calculation such as QMC is performed and the results are compared. It is hoped that our results at a very small superfluid fraction can at least give a good qualitative picture of the system.

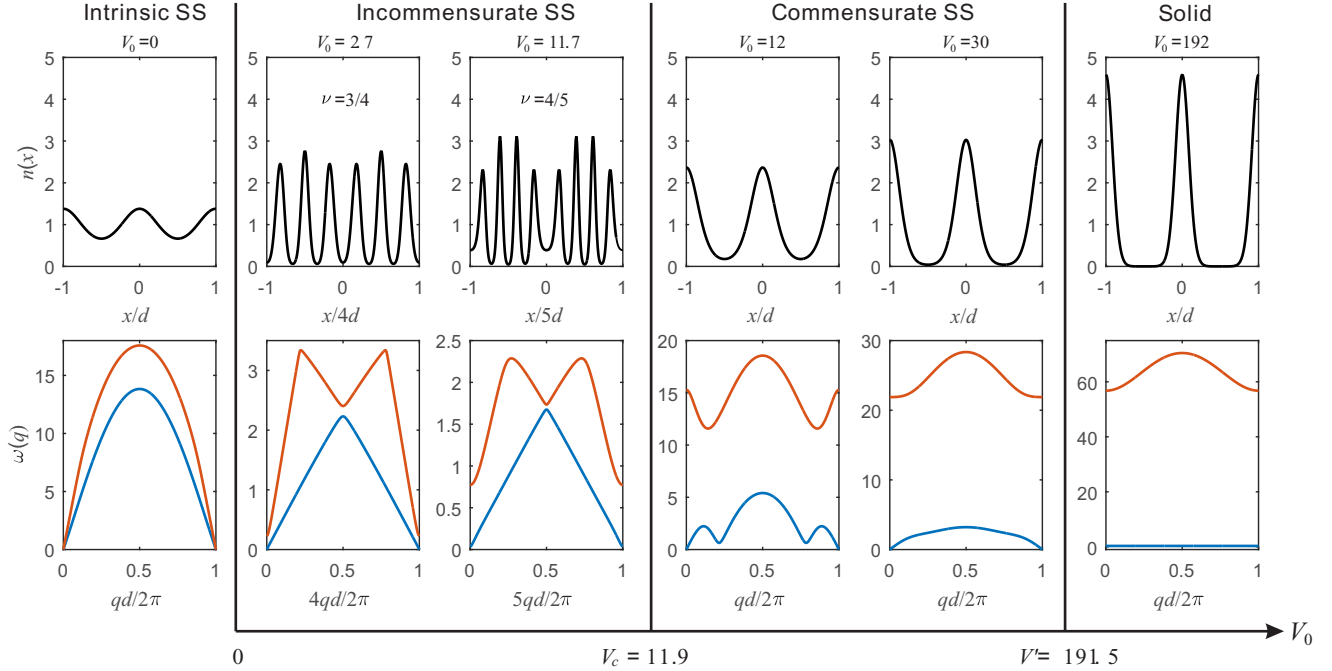


FIG. 1. Representatives of the ground-state density distributions $n(x)$ vs space x (top row) and lowest two excitation modes $\omega(q)$ vs wave vector q in a reduced zone scheme (bottom row) for various supersolid and solid states of a 1D soft-core interacting ultracold Bose gas in a lattice potential $V(x) = V_0 \sin^2(\pi x/d)$. d is the lattice constant, and see text for other parameters. From the second left column to the right column correspond, respectively, to $\nu = 3/4$ incommensurate SS ($V_0 = 2.7$), $\nu = 4/5$ incommensurate SS ($V_0 = 11.7$), commensurate SS ($V_0 = 12$), commensurate SS ($V_0 = 30$), and the solid ($V_0 = 192$). $n(x)$, $\omega(q)$, and V_0 are respectively in units of $1/d$, \hbar/md^2 , and \hbar^2/md^2 with m the atom mass.

In a log - log scale, we show the velocities v_1, v_2 and the gap Δ as a function of lattice depth V_0 in Fig. 2. In Fig. 2(a) of v_1 vs V_0 , there appears a jump of v_1 at $V_0 = V_c$ responsible for the incommensurate-to-commensurate SS transition. The drastic drop of v_1 at $V_0 = V' = 191.5$ corresponds to where the SS-to-solid transition is. Superfluidity is completely suppressed at this point. In Fig. 2(b) of v_2 vs V_0 , the peak down from $v_2 \rightarrow 0$ is where ω_2 with a downward feature ($\omega_2^2 = \Delta^2 - v_2^2 q^2$) shifts to the one with an upward feature ($\omega_2^2 = \Delta^2 + v_2^2 q^2$). For onset at V_c , the downward ω_2 occurs as a companion of a roton emerging in the lowest mode. In Fig. 2(c) of Δ vs V_0 , a large Δ jump is seen at V_c that again signals the incommensurate-to-commensurate SS transition. It is interesting to note that in the commensurate SS regime ($V_c \leq V_0 \leq V'$), a power law $\Delta = \Delta_0 V_0^\beta$ seems to occur with $\beta \approx 1/2$ and $\Delta_0 \simeq 4$. Similarly, in the $\nu = 3/4$ incommensurate SS regime, a power law $\Delta = \Delta'_0 V_0^{\beta'}$ occurs with $\beta' \approx 3/2$ and $\Delta'_0 \simeq 1/20$. The extrapolation implies that $\Delta \rightarrow 0$ when $V_0 \rightarrow 0$.

IV. A VARIATIONAL STUDY

To shed more light on the excitation physics of a soft-core interacting SS system, we also perform a variational computation on ω_1 in the tight-binding (commensurate) regime ($V_c \leq V_0 \leq V'$). One important constraint for choosing the trial wave function is to generate a good match for the superfluid fraction f_s . For a lattice system in the tight-binding regime, f_s is mainly determined by the tunneling energy in the potential barrier region. It was shown that $f_s = m/m^* = -2d^2[\psi(x)d\psi(x)/dx]_{x=d/2}$, with $\psi(x)$ the corre-

sponding wave function [32]. It turns out that a Gaussian ansatz $|\psi(x)|^2 = A \exp(-Cx^2)$ with $A = \tilde{V}_0^{1/4}/4d$ and $C = (\tilde{V}_0\pi^2)^{1/2}/d^2$ ($\tilde{V}_0 \equiv md^2V_0/\hbar^2$ is a dimensionless quantity) which reproduces well the density distribution in the potential barrier region can lead to a good fit for f_s . Consequently, one obtains

$$f_s = \frac{\pi \tilde{V}_0^{3/4}}{4} \exp\left(-\frac{\pi \tilde{V}_0^{1/2}}{4}\right). \quad (6)$$

As shown in Fig. 3(a), the analytic f_s in (6) is compared to the one from the exact numerical calculation. The latter is obtained by first solving the lowest Bloch band $E_1(k)$ of the system and then taking $f_s = m/m^* = \lim_{k \rightarrow 0} m/\hbar^2[\partial^2 E_1(k)/\partial k^2]$ [18,34]. A good match is seen between the two f_s 's. It should be noted that the superfluid fraction being exactly equal to the inverse effective mass holds only within the mean-field Gross-Pitaevskii approach. For strong interacting systems, the relation is not necessarily correct.

We next derive the corresponding hydrodynamic equations based on the time-dependent GPE. With $\psi(x,t) = \sqrt{n(x,t)}e^{i\phi(x,t)}$ and considering the density and phase fluctuations: $n(x,t) \equiv n_0(x) + \delta n(x,t)$ and $\phi(x,t) \equiv \phi_0(x) + \delta\phi(x,t)$ with $\phi_0(x) \equiv 0$, we obtain, after some algebra,

$$\partial_t^2 \delta n = -\partial_x \left\{ \frac{\hbar^2}{4mm^*} n_0 \partial_x \left[\frac{\partial_x^2 \delta n}{n_0} - \frac{\partial_x^2 n_0 \delta n}{n_0^2} - \frac{\partial_x n_0 \partial_x \delta n}{n_0^2} + \frac{(\partial_x n_0)^2 \delta n}{n_0^3} \right] - \frac{n_0}{m^*} \partial_x \int U(\bar{x}) \delta n(x',t) dx' \right\}. \quad (7)$$

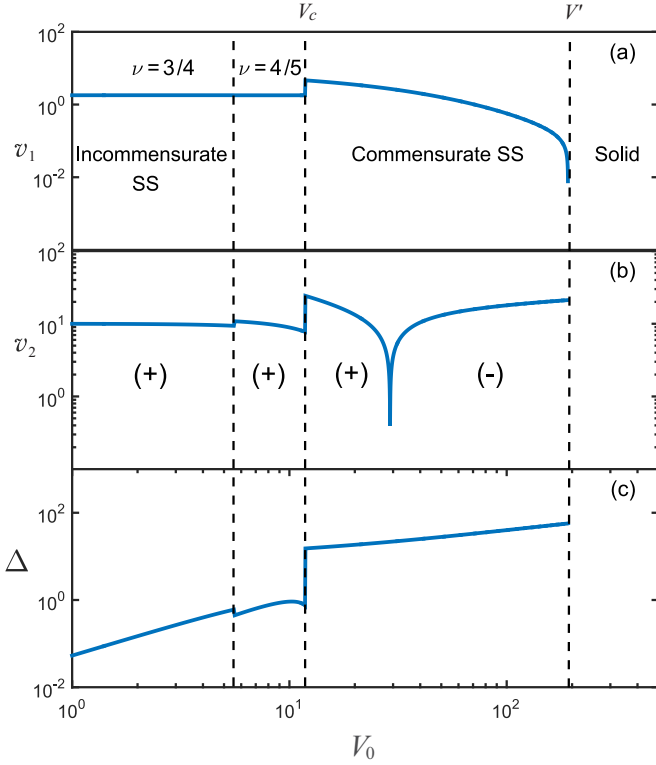


FIG. 2. In log-log scales, sound velocity v_1 in ω_1 and sound velocity v_2 and gap Δ in ω_2 are shown, respectively, as a function of lattice depth V_0 . In (b), the peak down separates ω_2 with a downward (-) or an upward (+) feature (see text). v_1 and v_2 are in units of \hbar/md and Δ and V_0 are in units of \hbar^2/md^2 .

By Fourier expansions $\delta n(x,t) = (1/2\pi) \int dq \delta n_q \exp(iqx - i\omega_1 t)$ and $\partial_x^n \delta n(x,t) = (1/2\pi) \int dq (iq)^n \delta n_q \exp(iqx - i\omega_1 t)$ and using the Gaussian ansatz to construct the periodic $n_0(x) = \bar{n}_0 \sum_j |2\psi(x - jd)|^2$, we obtain at low q

$$\omega_1^2 = \frac{q^2}{2m^*} \left[\frac{\hbar^2 q^2}{2m} + 2\bar{n}_0 \tilde{U}(q) - \frac{\pi \sqrt{\tilde{V}_0}}{md^2} - \frac{\pi \tilde{V}_0}{12md^2} \right], \quad (8)$$

where $\tilde{U}(q)$ is Fourier component of $U(x)$. To obtain the analytic dispersion in (8), the tails of each Gaussian wave packet that extend to neighboring sites have been neglected in $n_0(x)$. Substituting the result in (6) into (8), one obtains at $q \rightarrow 0$

$$v_1^2 = \frac{\pi \tilde{V}_0^{3/4}}{4m} e^{-\frac{\pi \sqrt{\tilde{V}_0}}{4}} \left[\bar{n}_0 \tilde{U}(0) - \frac{\pi \sqrt{\tilde{V}_0}}{2md^2} - \frac{\pi \tilde{V}_0}{24md^2} \right]. \quad (9)$$

Equation (9) is valid for $v_1^2 \geq 0$. Figure 3(b) shows a good agreement between the analytic v_1 in (9) and the exact numerical v_1 already shown in Fig. 2(a).

Elementary excitation of a uniform short- or long-range SF system can be described as $\omega^2 = (q^2/2m)[(q^2/2m) + 2\bar{n}_0 U(q)]$, with $U(q)$ the Fourier transform of the interaction. Comparing it with the result in (8), one sees explicitly how the lattice potential affects the lowest excitation of the lattice SF/SS system at the tight-binding regime. In fact, the

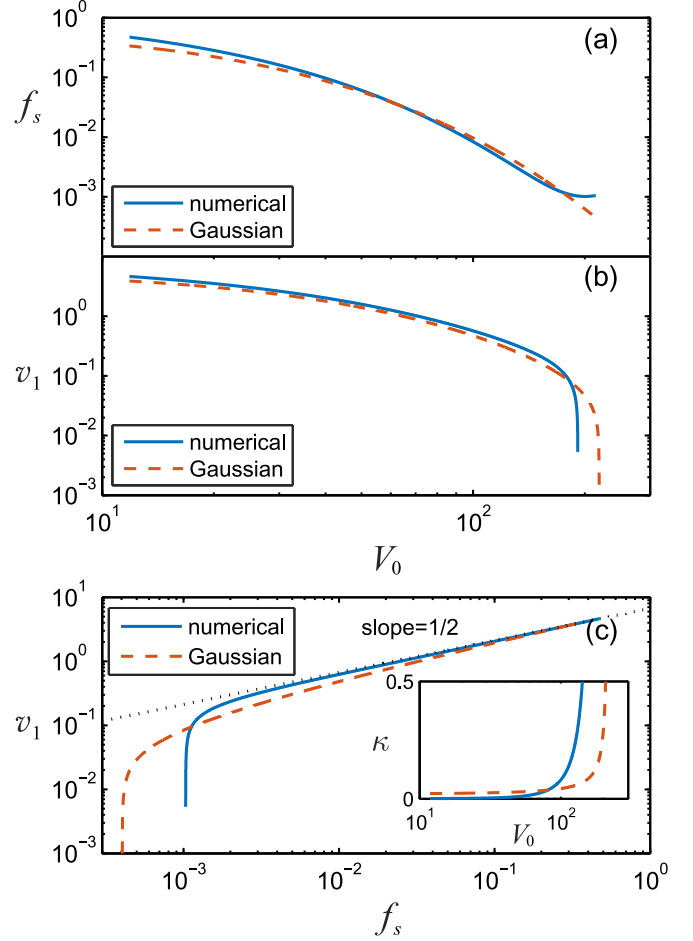


FIG. 3. Comparisons of superfluid fraction f_s vs V_0 [(a)] and phonon velocity v_1 vs V_0 [(b)] obtained by variational (dashed red line) and exact numerical (solid blue line) calculations. Frame (c) shows the power law $v_1 \sim \sqrt{f_s}$ for a large span of V_0 . The inset shows that the compressibility κ remains constant for a large span of V_0 and diverges at the SS-to-solid transition. v_1 is in units of \hbar/md , V_0 is in units of \hbar^2/md^2 , and κ is in units of md^2/\hbar^2 .

additional two terms associated with V_0 in (8) can be ascribed to the quantum-pressure effect induced by the structure of the ground state.

Finally, in Fig. 3(c) we compare v_1 with f_s for both variational and exact numerical results. In both curves, the power law $v_1 \sim \sqrt{f_s}$ remains valid for a large range of V_0 for the present soft-core system. The lines deviate and drop significantly at some high V_0 , indicating that the system is entering the solid state. At this point the compressibility $\kappa = f_s/mv_1^2 \rightarrow \infty$ (see the inset).

V. CONCLUSION

In conclusion, excitations of a 1D ultracold soft-core interacting Bose gas with optical lattices are theoretically investigated. Characteristics and dispersions of the lowest two modes are shown for various supersolid and solid states. The power law $v_1 \sim \sqrt{f_s}$ with v_1 the velocity of the lowest phonon mode and f_s the superfluid fraction is identified in the current

system at the tight-binding regime. A final remark is that under the effect of a lattice potential, a strong soft-core interacting SF/SS system can sustain the superfluidity for a large range of V_0 . In contrast, superfluidity could be more easily depleted by lattice in a short-range system.

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