Sound speed of a Bose-Einstein condensate in an optical lattice

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The speed of sound of a Bose-Einstein condensate in an optical lattice is studied both analytically and numerically in all spatial three dimensions. Our investigation shows that the sound speed depends strongly on the strength of the lattice. In the one-dimensional case, the speed of sound falls monotonically with increasing lattice strength. The dependence on lattice strength becomes much richer in two and three dimensions. In the two-dimensional case, when the interaction is weak, the sound speed first increases and then decreases as the lattice strength increases. For the three-dimensional lattice, the sound speed can even oscillate with the lattice strength. These rich behaviors can be understood in terms of compressibility and effective mass. Our analytical results in the limit of weak lattices also offer an interesting perspective to help with our understanding: they show that the lattice component perpendicular to the sound propagation increases the sound speed while the lattice component parallel to the propagation decreases the sound speed. The various dependences of the sound speed on the lattice strength are the result of this competition.

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I. INTRODUCTION

A Bose-Einstein condensate (BEC) in an optical lattice has recently attracted great interest both experimentally and theoretically [1,2]. The presence of a lattice can remarkably enrich the behaviors of the system compared to the uniform case, providing fertile ground for exploring a variety of solid-state effects in BECs—for example, Bloch oscillations [3–5] and Landau-Zener tunneling [6–10] between Bloch bands in an accelerating optical lattice. Moreover, a BEC in an optical lattice can be considered as a quantum simulator and therefore used for testing fundamental theoretical concepts [2]. For example, it can be used to simulate the Bose-Hubbard model and study experimentally the quantum phase transition between a superfluid and Mott insulator [10,11].

In this article, we launch a systematic study of the speed of sound for a BEC in an optical lattice in all spatial three dimensions. The speed of sound is important for two simple reasons: (a) it is a basic physical parameter that tells how fast the sound propagates in the system, and (b) it is intimately related to superfluidity according to Landau's theory of superfluids. Because of these, the sound propagation and its speed were one of the first things that have been studied by experimentalists on a BEC since its first realization in 1995 [12]. The propagation of sound in a harmonically trapped condensate without a lattice has already been observed experimentally [13,14] and studied theoretically [15–20]. Now there are experimental efforts to measure the sound speed for a BEC in an optical lattice [22].

There has been a great deal of theoretical work done to understand the sound speed for a BEC in an optical lattice. These studies show that three parameters strongly affect the speed of sound: the strength of the optical lattice, v; the interaction between atoms, c; and the lattice dimension D ($D=1,2,3$) [21]. In Ref. [23], the phonon excitations of the BECs in a one-dimensional optical lattice ($D=1$) were theoretically investigated by solving the Bogoliubov equations. Their analytical results for the sound speed in the weak potential limit predicted that the sound speed decreases monotonically with increasing depth of the optical lattice. The most detailed study of sound propagation in one-dimensional (1D) lattices was done by Stringari and co-workers [24,25], who also found that the sound speed is suppressed by the lattice. In particular, Ref. [24] presents a detailed comparison between the sound speed obtained by the Bogoliubov theory and the one obtained from the compressibility and the effective mass. Similar results [26] were also obtained for the Krönig-Penney potential, a special form of the periodic potential. Furthermore, Martikainen and Stoof [27] examined the effect of the transverse breathing mode on the longitudinal sound propagation for a BEC in a one-dimensional optical lattice. In particular, they discussed how the coupling with the transverse breathing mode influences the sound velocity in an optical lattice. Krämer *et al.* [28] also studied the effect of the transverse degrees of freedom on the velocity of sound of a BEC in a 1D optical lattice and radially confined by a harmonic trap. A recent paper by Taylor and Zaremba [29] studied the Bogoliubov excitations of a BEC in an optical lattice in all spatial dimensions. However, in the formulation in Ref. [29] the authors did not present the concrete results of sound speed in the two- and three-dimensional cases ($D=2,3$). Most interestingly, with numerical calculations Boers *et al.* [30] found that the sound speed of a BEC in a three-dimensional optical lattice achieves a maximum with increasing lattice depth. Because of the difficulty to obtain the Bloch states with interaction, the investigation of Boers *et al.* is limited to low density so that the Bloch wave function of the free particle can be used as an approximation.

Our investigation here tries to overcome the deficiencies in previous studies to give a complete picture of how the sound speed is affected by the lattice strength v; the interaction between atoms, c; and the dimensionality D. Analytical approaches are used in two limiting cases: weak lattices and strong lattices. For weak lattices, they can be viewed as perturbations. In this case, we obtain an analytical expression to the second order of the lattice strength for the sound speed of a BEC in an *arbitrary periodic potential*. We have analyzed this result for the important case of the periodic potential being an optical lattice. Our analysis finds a strong dependence of the sound speed on the lattice dimensions. Especially, we find that the lattice component perpendicular to the sound propagation increases the sound speed while the lattice components parallel to the propagation suppresses the sound speed. Since the lattice can only be parallel to the propagation direction of sound in one-dimensional ($D=1$) optical lattices, the sound speed falls monotonically with increasing lattice strength. In two- and three-dimensional ($D=2,3$) optical lattices, there are both perpendicular and parallel components in the lattice and, therefore, there is competition. As a result, there is a rich dependence of the sound speed on lattice strength in the case of $D=2,3$. The sound speed can first increase and then decrease as the lattice strength increases. We have also tried to understand these results from a different angle—i.e., in terms of compressibility κ and effective mass m^*. The analytical expression is found for compressibility κ and effective mass m^* for a BEC in an optical lattice. We find that the effect of the lattice on the sound speed reflects competition between the slowly decreasing compressibility κ and the increasing effective mass m^* with increasing lattice depth.

In the limit of strong lattices, it is reasonable to use the tight-binding model to describe the BEC of dilute density in an optical lattice [31]. Our analytical results display that the sound speed always exponentially decreases with the increase of lattice strength, independent of dimension D. This universal behavior of sound speed is the result of the competition between the tunneling strength J between adjacent sites and the interaction U between the atoms at a lattice site: with the increase of lattice depth, U slowly increases while J exponentially decreases.

Our analytical results are complemented by our numerical study, where the results are obtained for all ranges of lattice strength. Our numerical results agree well with our analytical results both in weak potential and tight-binding limits for the case of weak interatomic interaction. For the intermediate strength of lattices, we find that the sound speed even oscillates with the lattice strength for a three-dimensional optical lattice. We emphasize that in our numerical calculations the interaction between atoms is taken into account to compute the Bloch states in all three dimensions. In Ref. [30], the interaction is neglected in computing Bloch states for BECs and the Bloch states of free bosons were used as an approximation.

This paper is organized as follows. In Sec. II, for the sake of self-containment and introducing the notation, we describe the basic theoretical framework of our study. It includes the definition of the sound speed v_s, compressibility κ, and effective mass m^*. In Sec. III, we present the analytic results of the sound speed for a BEC in the optical lattice in both the weak potential limit and tight-binding regime. Section IV contains our numerical study of the sound speed. The details of our numerical methods are given there. In Sec. V, we discuss the possibility of observing the phenomena presented in this paper within the current experimental capability. The last section (Sec. VI) contains a discussion of our results and concluding remarks. Five appendixes are given at the end to show the detailed steps to derive our key analytical results in the main text.

II. BASIC THEORY

A. Mean-field theory of Bose-Einstein condensates

We focus on the situation that the BEC system can be well described by mean-field theory. In this case, the BEC system is governed by the following grand-canonical Hamiltonian [1]:

$$\mathcal{H} = \int d^3\vec{r}\left\{\psi^*(\vec{r})\left[-\frac{1}{2}\nabla^2 + V_{latt}(\vec{r})\right]\psi(\vec{r}) + \frac{c}{2}|\psi(\vec{r})|^4 - \mu|\psi(\vec{r})|^2\right\}. \tag{1}$$

In our case, the external potential is a three-dimensional optical lattice created by six laser beams that are perpendicular to each other [1,2]:

$$V_{latt}(\vec{r}) = v[\cos(x) + \cos(y) + \cos(z)], \tag{2}$$

where v characterized the strength of the optical lattice. In Eq. (1), all variables are scaled to be dimensionless by the system's basic parameters: the atomic mass m, the wave number k_L of the laser light, and the average density n_0. The chemical potential μ and the strength v of the periodic potential are in units of $4\hbar^2k_L^2/m$, the wave function ψ is in units of $\sqrt{n_0}$, and $\vec{r}$ is in units of $1/2k_L$. The nonlinear coefficient $c=\pi n_0 a_s/k_L^2$, where $a_s>0$ is the s-wave scattering length. In this article, the parameters c and v in Eq. (1) relate to the parameters gn_0/E_R and V_{opt}/E_R, which are often used in the literature [1], as $c=gn_0/8E_R$ and $v=V_{opt}/16E_R$ with $E_R=\hbar^2k_L^2/2m$.

Sound is a propagation of low-density fluctuations inside a system. To study sound in a BEC, one first needs to find out the ground state of this BEC system, which serves as a medium for sound propagation. The sound speed can then be found by perturbing the ground state as explained in detail in the next subsection.

The ground state of a BEC in an optical lattice is a Bloch state at the center of the Brillouin zone. Briefly, the Bloch state is of the form

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\phi_{\vec{k}}(\vec{r}), \tag{3}$$

where $\vec{k}$ is the Bloch wave vector and $\phi_{\vec{k}}(\vec{r})$ is a periodic function with the same periodicity of the optical lattice. The Bloch wave function $\phi_{\vec{k}}(\vec{r})$ satisfies the stationary Gross-Pitaevskii equation

$$-\frac{1}{2}(\vec{\nabla} + i\vec{k})^2\phi_{\vec{k}} + c|\phi_{\vec{k}}|^2\phi_{\vec{k}} + V_{latt}(\vec{r})\phi_{\vec{k}} = \mu(\vec{k})\phi_{\vec{k}}, \tag{4}$$

where $\mu(\vec{k})$ is the chemical potential. The energy of the system in a Bloch state is given by

$$E(\vec{k}) = \int d^3\vec{r}\left\{ \phi_{\vec{k}}^{*}\left[-\frac{(\vec{\nabla}+i\vec{k})^2}{2} + V_{latt}(\vec{r}) \right]\phi_{\vec{k}} + \frac{c}{2}|\phi_{\vec{k}}|^4 \right\}. \tag{5}$$

The set of energies $E(\vec{k})$ then forms a Bloch band [32,33]. The Bloch state can be obtained analytically in certain circumstances [34]. In most cases, it has to be computed numerically [32,35]. The numerical method of this study is described in Sec. VI. To compute the sound speed, one may only need the Bloch state ϕ_0 at $\vec{k}=0$. However, for the effective mass tensor defined by [29,36]

$$\left(\frac{1}{m^*}\right)_{\alpha,\beta} = \left(\frac{\partial^2 E(\vec{k})}{\partial k_\alpha \partial k_\beta}\right)_{k=0}, \tag{6}$$

where $k=|\vec{k}|$ and $\alpha,\beta=x,y,z$, one has to compute Bloch states in the vicinity of $\vec{k}=0$. We also study one- and two-dimensional cases. The one-dimensional optical lattice is given by

$$V(x) = v\cos(x), \tag{7}$$

and the two-dimensional optical lattice is given by

$$V(x,y) = v[\cos(x)+\cos(y)]. \tag{8}$$

B. Definitions of the sound speed

In Sec. II A, the BEC system is regarded as a Hamiltonian system by the grand canonical Hamiltonian (1); the corresponding time-dependent Gross-Pitaevskii equation can be obtained by the variation of the Hamiltonian, $i\partial\psi/\partial t = \delta H/\delta\psi^*$,

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\nabla^2\psi + V(\vec{r})\psi + c|\psi|^2\psi. \tag{9}$$

In Eq. (9), the time t is the units of $m/4\hbar k_L^2$. The Bogoliubov equations can be determined from the linear stability analysis of the GP equation (9). To explore a small disturbance $\delta\phi_{\vec{k}}(\vec{r},t)$ at a Bloch state $\phi_{\vec{k}}(\vec{r})$, we write

$$\psi(\vec{r},t) = e^{i\vec{k}\cdot\vec{r}-i\mu t}[\phi_{\vec{k}}(\vec{r}) + \delta\phi_{\vec{k}}(\vec{r},t)], \tag{10}$$

where the disturbance can be similarly written as

$$\delta\phi_{\vec{k}}(\vec{r},t) = u_{\vec{k}}e^{i\{\vec{q}\cdot\vec{r}-\epsilon(\vec{q})t\}} + v_{\vec{k}}^{*}e^{-i\{\vec{q}\cdot\vec{r}-\epsilon(\vec{q})t\}}. \tag{11}$$

Plugging Eq. (11) into Eq. (9) and keeping only the linear terms, we arrive at the Bogoliubov equations [32],

$$\delta_z M_{\vec{k}}(\vec{q})\begin{pmatrix} u_{\vec{k}} \\ v_{\vec{k}} \end{pmatrix} = \epsilon(\vec{q})\begin{pmatrix} u_{\vec{k}} \\ v_{\vec{k}} \end{pmatrix}, \tag{12}$$

with

$$M_{\vec{k}}(\vec{q}) = \begin{pmatrix} \mathcal{L}(\vec{k}+\vec{q}) & c\phi_{\vec{k}}^2 \\ c\phi_{\vec{k}}^{*2} & \mathcal{L}(-\vec{k}+\vec{q}) \end{pmatrix} \tag{13}$$

and

$$\delta_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{14}$$

where $\mathcal{L}(\vec{q})$ is defined as

$$\mathcal{L}(\vec{q}) = -\frac{1}{2}(\vec{\nabla}+i\vec{q})^2 + V(\vec{r}) - \mu + 2c|\phi_{\vec{k}}|^2. \tag{15}$$

Note that $\vec{q}$ represents the mode of the small perturbations and is of the nature of a Bloch wave vector as the matrix M is periodic.

In general, there are two equivalent definitions for the sound speed in a BEC. As sound can be regarded as a long-wavelength response of a system to a perturbation, the sound speed can be extracted from the excitation of a BEC. According to the Bogoliubov theory, the excitation energy $\epsilon(\vec{q})$ of the BEC in a Bloch state at $\vec{k}=0$ can be found by solving the eigenvalue problem of Eq. (12). In this paper, we only consider the propagation of sound along one of the axes of the optical lattice. In terms of the excitations, the sound speed of a BEC system can be defined as

$$v_{s,i} = \lim_{q\to 0}\frac{\epsilon(\hat{q}_i)}{q}, \tag{16}$$

where $q=|\hat{q}_i|$ and $\hat{q}_i$ is a vector along the i axis ($i=x,y,z$).

The other definition arises when the BEC system is regarded as a hydrodynamics system. In this context, the sound speed along the i axis ($i=x,y,z$) in a BEC is given by the standard expression [24,25,37]

$$v_{s,i} = \sqrt{\frac{1}{\kappa m_i^*}}, \tag{17}$$

where the diagonal element m_i^* of the effective mass is defined by $m_i^* = d^2E/dk_i^2$ ($i=x,y,z$) and κ is the compressibility of the BEC system, defined as

$$\kappa^{-1} = n_0\frac{\partial\mu}{\partial n_0}, \tag{18}$$

where the chemical potential μ and n_0 is the averaged density. For a BEC system with repulsive interatomic interaction, the optical trapping reduces the compressibility of the system as the effect of the repulsion is enhanced by squeezing the condensate in each well. According to the definition of sound speed in Eq. (17), the sound speed reflects the competition between the compressibility κ and the effective mass m^*.

Both definitions are used in our computations, and they agree with each other as expected. The proof of the equivalence of these definitions can be found in Refs. [29,37].

III. ANALYTICAL RESULTS

A. Weak potential limit

We consider first an arbitrary periodic potential $V_{ar}(\vec{r})$ with the periodicity of $\vec{R}$,

$$V_{ar}(\vec{r}) = V_{ar}(\vec{r}+\vec{R}), \tag{19}$$

with

$$\vec{R} = m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3, \tag{20}$$

where $\vec{r}$ is the position vector, $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ are the three primitive vectors, and m_1, m_2, m_3 range through all integral values. In the weak potential limit, the periodic potential $V_{ar}(\vec{r})$ can be regarded as a perturbation. This allows us to solve both the Gross-Pitaevskii equation (4) and the Bogoliubov eigenvalue problem (12) perturbatively by expanding the wave function ψ and chemical potential μ of the BEC system in the order of the weak potential,

$$\psi = \psi^{(0)} + \psi^{(1)} + \psi^{(2)} + \cdots,$$

$$\mu = \mu^{(0)} + \mu^{(1)} + \mu^{(2)} + \cdots, \tag{21}$$

where $\psi^{(0)}$ and $\mu^{(0)}$ are the zeroth order of the potential strength, $\psi^{(1)}$ and $\mu^{(1)}$ the first order, etc. We find that the sound velocity along a given direction indicated by a unit vector $\hat{r}$ is

$$v_s = \sqrt{c} + 8\sqrt{c}\sum_{\vec{n}\neq 0}\left\{\frac{|\vec{n}|^2}{(4c+|\vec{n}|^2)^3} - \frac{|\vec{n}\cdot\hat{r}|^2}{|\vec{n}|^2(4c+|\vec{n}|^2)^2}\right\}\mathcal{F}_{\vec{n}}^2(V). \tag{22}$$

We emphasize that Eq. (22) is an expression of the sound speed along an arbitrary direction—i.e., not just along one of the axes of the optical lattice. In Eq. (22), $\mathcal{F}_{\vec{n}}(V)$ is the Fourier coefficient of $V_{ar}(\vec{r})$ as defined by

$$\mathcal{F}_{\vec{n}}(V) = \frac{1}{\Omega}\int_{cell} d^3\vec{r}\, V_{ar}(\vec{r})e^{-i\vec{n}\cdot\vec{r}}, \tag{23}$$

with

$$\vec{n} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3, \tag{24}$$

where n_j's are integers and $\vec{b}_j$'s are the set of reciprocal primitive vectors defined by

$$\vec{a}_i\cdot\vec{b}_j = 2\pi\delta_{ij}. \tag{25}$$

In the integration, Ω is the volume of the primitive cell and the integration is over one primitive cell. The detailed derivation of Eq. (22) can be found in Appendix C.

The focus of this article is optical lattices as described in Eqs. (2), (7), and (8). In this special but important case, the primitive vectors $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ can be chosen along the directions of the laser beams, $\vec{x}$, $\vec{y}$, and $\vec{z}$, respectively. Also we have $|\vec{a}_1| = |\vec{a}_2| = |\vec{a}_3| = 2\pi$. For this case, we find from Eq. (22) that if the sound propagation direction is along the x axis, the sound speed is [see also Eq. (C10) in Appendix C or Eq. (D43) in Appendix D]

$$v_{s,x} = \sqrt{c} + \sum_{\vec{n}\neq 0}\frac{8\sqrt{c}[(n_2^2+n_3^2)|\vec{n}|^2 - 4cn_1^2]}{|\vec{n}|^2(4c+|\vec{n}|^2)^3}\mathcal{F}_{\vec{n}}^2(V). \tag{26}$$

The sound speeds along the y and z axes can be found easily with permutation argument and the sound speed along a general direction is a certain combination of these three speeds.

When there is no periodic potential $V_{ar}(\vec{r})=0$, the sound speed in Eq. (26) is reduced to $\sqrt{c}$, the sound speed for a BEC in free space, as expected. We also notice that there is no first-order correction to the sound speed due to the periodic potential. Most importantly, the analytical result in Eq. (26) reveals that the lattice component perpendicular to the sound propagation (generated by the laser beams along the y and z axes) increases the sound speed while the lattice components parallel to the propagation (generated by the laser beams along the x axis) decreases the sound speed. As a result of this competition, the sound speed can either increase or decrease with lattice strength. This competition between the parallel and perpendicular components of the optical lattice certainly also applies to a general periodic potential if one carefully examines Eq. (22) and interprets "parallel" and "perpendicular" in a more general sense.

To illustrate this more clearly, we consider a simple case where the periodic potential is a 1D optical lattice given by $V_{ex}(\vec{r}) = v\cos(y)$. There are only two nonvanishing Fourier coefficients: i.e., $\mathcal{F}_{0,1,0}(V) = \mathcal{F}_{0,-1,0}(V) = v/2$. Then according to Eq. (26), the speeds of sound along the x, y, and z axes read, respectively,

$$v_{s,x} = v_{s,z} = \sqrt{c}\left(1 + \frac{v^2}{2\left(2c+\frac{1}{2}\right)^3}\right),$$

$$v_{s,y} = \sqrt{c}\left(1 - \frac{2cv^2}{\left(2c+\frac{1}{2}\right)^3}\right), \tag{27}$$

which show that with increasing the strength of the optical lattice the sound speed along the y axis, parallel to the periodic lattice, falls while the speeds of sound along both the x and z axes increase.

Now we study the BEC sound speed in optical lattices in terms of compressibility and effective mass according to the second definition of speed of sound: i.e., Eq. (17). Again we treat the weak optical lattice as a perturbation. For optical lattices of all dimensions as described in Eqs. (2), (7), and (8), we find the chemical potential at $\vec{k}=0$,

$$\mu = c - \frac{Dv^2}{4\left(2c+\frac{1}{2}\right)^2}, \tag{28}$$

and the system energy near $\vec{k}=0$,

$$E(\vec{k}) = \frac{k^2}{2} - \frac{v^2}{(1+4c)^2(4k^2-1)}, \tag{29}$$

with $k^2 = \Sigma_{i=x,y,z}k_i^2$. So the chemical potential depends on D, the dimension of the lattice, while the energy $E(k)$ does not. The compressibility κ can be calculated from the chemical potential μ via Eq. (18), and it is given by

$$\kappa^{-1} = c + \frac{Dcv^2}{\left(\frac{1}{2}+2c\right)^3}. \tag{30}$$

This shows that the compressibility κ tends to decrease with increasing v as the optical lattice localizes the BECs inside each well. Moreover, the compressibility κ decreases faster with v for higher-dimensional lattices. The effective mass m^* can be computed from $E(\vec{k})$, and it is found that

$$\frac{1}{m_i^*} = \left(1 - \frac{2v^2}{\left(\frac{1}{2}+2c\right)^2}\right), \tag{31}$$

with $i=x,y,z$. It is clear that the effective mass always increases with the lattice strength v. This is expected as the increased lattice strength suppresses the tunneling between neighboring wells and thus increases the effective mass m^*. Interestingly, in contrast to the chemical potential μ, the dependence of the effective mass on v is independent of the lattice dimension D. As the speed of sound is defined as $v_s = \sqrt{1/(\kappa m^*)}$, the compressibility κ and the effective mass m^* influence the sound speed in opposite directions.

Plugging both Eqs. (30) and (31) into Eq. (17), we find an analytical expressions for the sound speed of a BEC in an optical lattice up to the second order of v:

$$v_{s,i} = \sqrt{c}\left(1 + \frac{4(D-1-4c)}{(4c+1)^3}v^2\right), \quad i=x,y,z. \tag{32}$$

With simple algebra [see Eq. (E6) in Appendix E], one can show that this expression is consistent with the more general formula in Eq. (26).

Equation (32) indicates that in one-dimensional ($D=1$) optical lattices, the effective mass m^* always wins over the compressibility κ, resulting in a decreasing sound speed with lattice strength. However, in two- or three-dimensional ($D=2,3$) optical lattices, the situation is very different. There exists a critical value of c, the interatomic interaction strength, beyond which the effective mass m^* wins. Otherwise, the compressibility κ has a greater influence on the speed of sound and the speed of sound increases as the lattice becomes stronger. The critical values are $c=1/4$ for $D=2$ and $c=1/2$ for $D=3$.

We have discussed the behavior of the speed of sound in two different languages: one in terms of perpendicular and parallel components of the periodic potential with Eq. (26) and the other in terms of effective mass m^* and compressibility κ. Are these two pictures consistent? The answer is yes. To see this, we rewrite Eq. (26) as

$$v_{s,x} = \sqrt{c} + 8\sqrt{c}\left\{\sum_{\vec{n}\neq 0}\frac{|\vec{n}|^2}{(4c+|\vec{n}|^2)^3} - \sum_{\vec{n}\neq 0}\frac{n_1^2}{|\vec{n}|^2(4c+|\vec{n}|^2)^2}\right\}\mathcal{F}_{\vec{n}}^2(V). \tag{33}$$

By comparing it with Eqs. (30) and (31), it is apparent that the first term in the curly brackets comes from the compressibility κ while the second term results from the effective mass m^*. This observation gives us the following picture: on the one hand, all components of the periodic potential contribute to the compressibility κ, which leads to an enhancement of the sound speed; on the other hand, only the component parallel to the sound propagation increases the effective mass m^*, which leads to a suppression of the sound speed. Since the effective mass m^* always wins over κ along the parallel direction, we come to the previous understanding: the perpendicular components increase the sound speed while the parallel one suppresses it.

B. Tight-binding regime

When the potential wells are sufficiently deep, the condensate is well localized at each lattice site and the following tight-binding model may become adequate to describe the BEC in an optical lattice [31]:

$$\mathcal{H} = -J\sum_{\langle\vec{n},\vec{n}'\rangle}(\psi_{\vec{n}}^*\psi_{\vec{n}'} + \psi_{\vec{n}'}^*\psi_{\vec{n}}) + \frac{U}{2}\sum_{\vec{n}}|\psi_{\vec{n}}|^4, \tag{34}$$

where the first summation is over all pairs of nearest neighbors. The tunneling constant J, which quantifies the microscopic tunneling rate between adjacent sites, is given by

$$J = -\frac{1}{(2\pi)^D}\int d^D\vec{r}\left[\frac{1}{2}(\vec{\nabla}\varphi_{\vec{n}}\cdot\vec{\nabla}\varphi_{\vec{n}+1}) + \varphi_{\vec{n}}V\varphi_{\vec{n}+1}\right], \tag{35}$$

with $\varphi_{\vec{n}}$ being the wave function localized at site $\vec{n}$. The on-site interaction as given by

$$U = \frac{c}{(2\pi)^D}\int d^D\vec{r}\varphi_{\vec{n}}^4 \tag{36}$$

is a measure of the interaction between atoms at one lattice site. The ground state of this Hamiltonian is a constant wave function $\psi_{\vec{n}}=1$. Its excitation energy is given by $\epsilon(q_x) = 2|\sin(q_x\pi)|\sqrt{2J_xU}$, which yield the sound speed via Eq. (16) along the x axis of the optical lattice:

$$v_{s,x} = \sqrt{8\pi^2 J_x U}. \tag{37}$$

This result is consistent with the sound speed definition in terms of compressibility κ and effective mass m^* [24] since

$$J_x = \frac{1}{8\pi^2}\frac{m}{m_x^*}, \quad U \approx \kappa^{-1}. \tag{38}$$

In the following, we try to express J and U in terms of c and v. For a state well localized at each lattice site, we can regard it as the ground state of the lattice well and describe the localized state $\varphi_{\vec{n}}$ with the ground-state wave function of a harmonic oscillator. This approximation immediately leads to an estimate of U. We obtain

$$U = c(4\pi^2 v)^{D/4}. \tag{39}$$

As $U \approx \kappa^{-1}$, this indicates that the compressibility in the tight-binding limit is very similar to the weak potential limit: it depends on the dimensionality of the lattice and decreases with v in a nonexponential form.

Mathematically, the time-independent Schrödinger equation for an atom in the cosine potential is a Mathieu equation. The theory of the Mathieu equation allows us to estimate J along the x axis of the optical lattice, which is given by [38,39]

$$J_x = \frac{4}{\sqrt{\pi}} v^{3/4} \exp[-8\sqrt{v}]. \tag{40}$$

This result is very different from the weak potential limit, where the effective mass $\frac{m_x^*}{m} = \frac{1}{8\pi^2 J_x}$ increases exponentially with $\sqrt{v}$. We emphasize that Eq. (40) is explicitly a single-particle result and only valid for weak interactions (see Fig. 8). As a result, J_x should dominate the behavior of the speed sound. Combining Eqs. (39) and (40), we arrive at

$$v_{s,x} = 2^{5/2}\pi^{3/4}c^{1/2}(4\pi^2 v)^{D/8} v^{3/8} \exp(-4\sqrt{v}), \tag{41}$$

which shows that the speed of sound decreases monotonically with v in an exponential form in all three dimensions. The sound speed in the tight-binding limit has a weak dependence on the dimension D of the lattice as D only appears in the prefactor of the exponential. We emphasize that Eqs. (39) and (40) are obtained by completely ignoring the interatomic interaction, so the analytical result of Eq. (41) will become invalid in the case of a strong interatomic interaction (or BECs of high density). After noticing the difficulty to obtain the analytical result on the boundary where Eq. (41) becomes invalid, we turn to a numerical effort. Later we shall discuss in detail how Eq. (41) becomes invalid with the numerical results on J_x (see Fig. 8).

IV. NUMERICAL RESULTS

We have so far studied analytically the sound speed of a BEC in an optical lattice. In this section, we study the sound speed with numerical methods. Our numerical method allows us to find the sound speed for the whole range of lattice strength, particularly the intermediate lattice strength for which no apparent analytical approach is available at present.

A. Numerical methods

As discussed in Sec. II, to compute the sound speed, one has to first find the ground state of the BEC system or the Bloch states in the vicinity of $\vec{k}=0$. To find these states numerically, we expand the Bloch states in a Fourier series

$$\phi_{\vec{k}}(\vec{r}) = \sum_{m,n,l=-N}^{N} a_{m,n,l} e^{i(mx+ny+lz)}, \tag{42}$$

where N is the cutoff. We find that $N=5$ is good enough for all dimensions. The Fourier coefficients $\{a_{m,n,l}\}$ satisfy the normalization condition

$$\sum_{m,n,l=-N}^{N} |a_{m,n,l}|^2 = 1. \tag{43}$$

Note that the Fourier coefficients $\{a_{m,n,l}\}$ can be chosen as real for our cases. This fact greatly reduces the computation burden.

The Bloch waves can be numerically obtained by varying $\{a_{m,n,l}\}$ so that the wave function $\phi_{\vec{k}}$ minimizes the system energy of Eq. (5); the accuracy is checked by substituting the solutions into the Gross-Pitaevskii equation (4). We use the standard minimization routine of MATLAB. The accuracy of

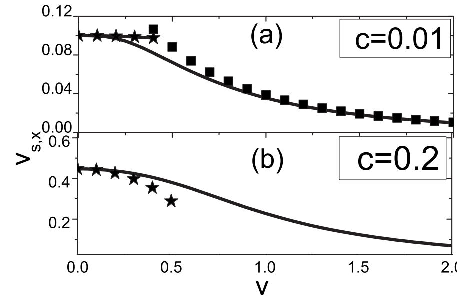

FIG. 1. Sound speed for a BEC in a 1D optical lattice via the strength of the optical lattice. The numerical results are denoted by the solid lines, analytical results for weak potentials by stars (★), and analytical tight-binding results by solid squares (■). Sound speed of $v_{s,x}$ is in units of $2\hbar k_L/m$, the nonlinear coefficient $c = \pi n_0 a_s/k_L^2$, and the lattice strength of v is in units of $4\hbar^2 k_L^2/m$.

the numerical solutions can be checked by substituting the numerical solutions into the time-independent Gross-Pitaevskii equation (4). Once the Bloch states $\phi_{\vec{k}}(\vec{r})$ have been obtained, we can compute the sound speed in two different methods. In one method, we calculate the Bogoliubov excitations $\varepsilon(q)$ of the ground state $\phi_0(\vec{r})$ and find the sound speed of the BEC through Eq. (16). In the other method, we can calculate the effective mass m_x^* and compressibility κ, respectively, with Eqs. (6) and (18). Then the sound speed can be computed via Eq. (17). We have calculated the sound speeds with both methods and the agreement is excellent as expected. We have reproduced the main results of Ref. [24] as a test of our numerical methods.

B. Results and discussion

We have computed numerically the sound speeds for all three dimensions for a wide range of lattice strength v and interatomic interaction c. The results are plotted in Figs. 1–3, respectively. Figure 1 displays the sound speed in the one-dimensional case, which falls monotonically with increasing

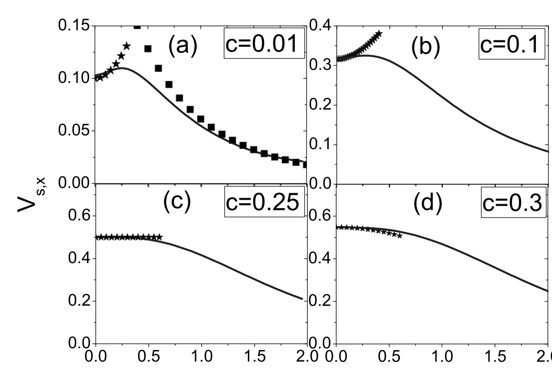

FIG. 2. Sound speed for a BEC in a 2D optical lattice via the strength of the optical lattice. The numerical results are denoted by the solid lines, analytical results for weak potentials by stars (★), and analytical tight-binding results by solid squares (■). Sound speed of $v_{s,x}$ is in units of $2\hbar k_L/m$, the nonlinear coefficient $c = \pi n_0 a_s/k_L^2$, and the lattice strength of v is in units of $4\hbar^2 k_L^2/m$.

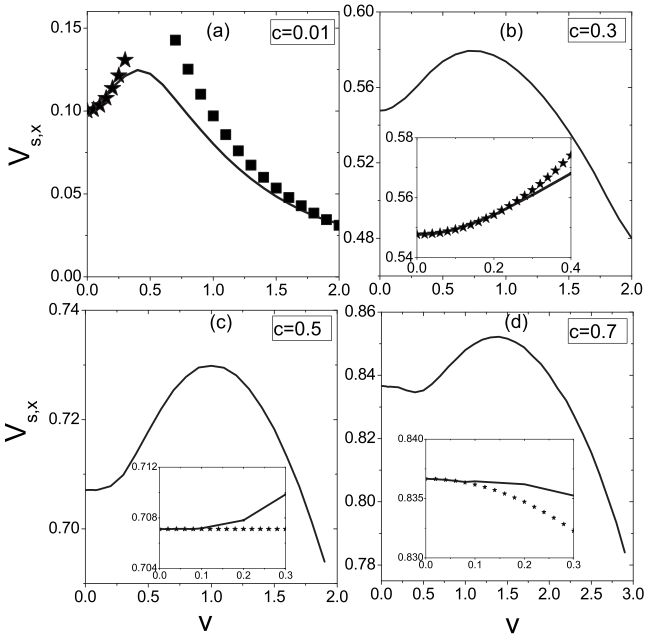

FIG. 3. Sound speed for a BEC in a 3D optical lattice via the strength of the optical lattice. The numerical results are denoted by the solid lines, analytical results for weak potentials by stars (⋆), and analytical tight-binding results by solid squares (■) curves. For clarity, the analytical results for weak potentials are compared to numerical result in the insets for $c=0.3$, $c=0.5$, and $c=0.7$. Sound speed of $v_{s,x}$ is in units of $2\hbar k_L/m$, the nonlinear coefficient $c=\pi n_0 a_s/k_L^2$, and the lattice strength of v is in units of $4\hbar^2 k_L^2/m$.

lattice strength. This is in agreement of previous studies [23–25].

The results are different in two and three dimensions. As shown in Figs. 2 and 3, the relationship between the sound speed and the lattice strength depends crucially on the strength of interatomic interaction. In the two-dimensional case, when the interaction is above the critical value—i.e., $c>\frac{1}{4}$—the speed of sound also decreases monotonically with increasing lattice strength [Fig. 2(d)]. However, when the interaction is weak—i.e., $c<\frac{1}{4}$—as shown in Figs. 2(a) and 2(b) the sound speed reaches a maximum at an intermediate strength of optical lattice. Figure 2(c) shows the transition point between the above two different behaviors, where the sound speed almost does not change with weak lattice potentials.

In three dimensions, the behavior becomes even richer. There exists a critical value of the interatomic interaction, $c=\frac{1}{2}$. When the interaction is smaller than this critical value ($c<\frac{1}{2}$), the sound speed first increases and then decreases as the lattice strength increases [Figs. 3(a)–3(c)]. This is similar to the two-dimensional case and was first noticed by Boers *et al.* [30]. However, when the interaction is strong enough—i.e., $c>\frac{1}{2}$—a new pattern is found. As shown in Fig. 3(d), the sound speed can even oscillate with the lattice strength. According to our numerical results, the oscillating behavior of the sound speed does not disappear until the interatomic interaction $c=1$.

The dependence of sound speeds on the lattice strength v is largely expected from our analytical results for the two limiting cases of weak and strong lattices. We have shown that in the weak lattice limit, the speed of sound can either increase or decrease with the lattice strength while in the strong lattice limit the speed of sound always decreases with increasing lattice strength. Naively, one would expect that the speed of sound either decreases monotonically with the lattice strength v or develops a maximum at a certain intermediate value of v. This is exactly what we have seen in Figs. 1–3 except in Fig. 3(d) where we see two local maxima.

Our numerical results are compared to our analytical results. As seen in Figs. 1–3, our numerical results agree very well with our analytical results [stars (⋆)] in the regime of weak potentials. For strong lattices, our numerical results also agree well with the tight-binding results [solid squares (■) in Figs. 1(a), 2(a), and 3(a)] for weak interactions. However, for strong interactions, there exists a large discrepancy between the tight-binding results and the numerical one. We shall discuss this in detail later.

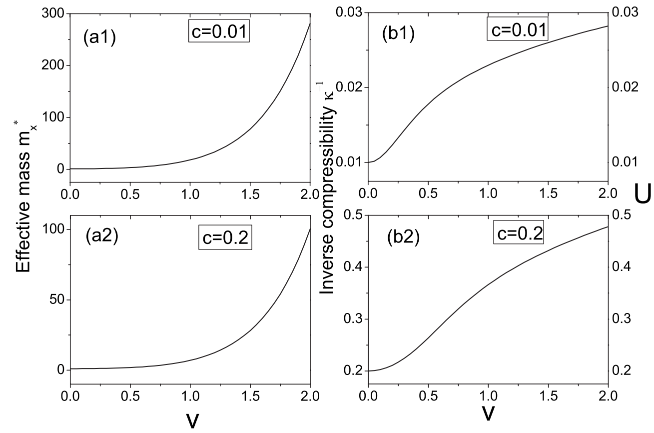

FIG. 4. Inverse compressibility κ^{-1} and effective mass m_x^* for a BEC in a 1D optical lattice via the strength of the optical lattice. Based on Eq. (38), U is equal to κ^{-1} in the tight-binding limit. The nonlinear coefficient $c=\pi n_0 a_s/k_L^2$, inverse compressibility κ^{-1} and U are in units of $4\hbar^2 k_L^2/m$, and the lattice strength v is in units of $4\hbar^2 k_L^2/m$.

To better understand the behavior of the sound speed as a function of the lattice strength v, we have also computed numerically the effective mass m_x^* and the compressibility κ and the results are plotted in Figs. 4–6. It is clear from these figures that the compressibility κ has different dependences on v in different dimensions. This agrees with our analytical results in the last section. However, we notice that the increasing rates of κ^{-1} with v are quite close in all dimensions.

The situation is different for the effective mass m_x^*. In the last section, we have shown that the effective mass m_x^* has the same dependence on v [see Eq. (31)] in all dimensions. However, it is true only in the limit of weak lattices. As seen in the right columns of Figs. 4–6, the effective mass m_x^*, as a function of v, behaves very differently in different dimensions. In particular, the increasing rate of m_x^* with v in one dimension is orders of magnitude larger than the increasing rate in three dimensions. The two-dimensional case is right in between. Since the sound speed is the result of the competition between m_x^* and κ, the relatively small increasing

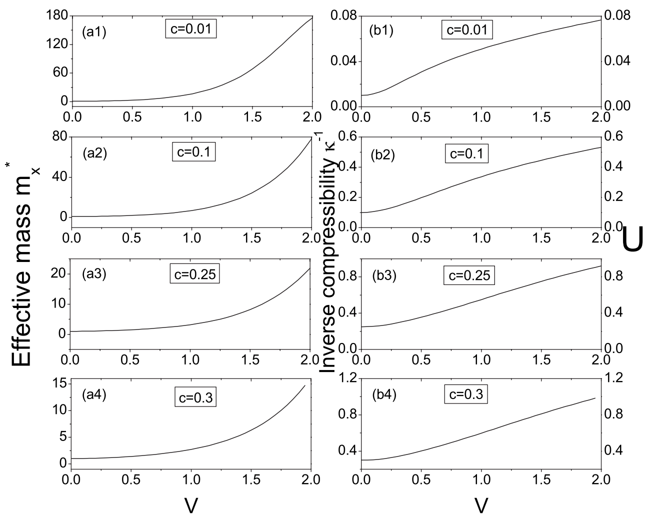

FIG. 5. Inverse compressibility κ^{-1} and effective mass m_x^* for a BEC in a 2D optical lattice via the strength of the optical lattice. Based on Eq. (38), U is equal to κ^{-1} in the tight-binding limit. The nonlinear coefficient $c=\pi n_0 a_s/k_L^2$, inverse compressibility κ^{-1} and U are in units of $4\hbar^2 k_L^2/m$, and the lattice strength v is in units of $4\hbar^2 k_L^2/m$.

rate of m_x^* with v allows the sound speed to oscillate with v in 3D.

In order to understand the interplay between the effects of the lattice dimensionality D and the interaction c on the effective mass, we plot it Fig. 7. As shown in Fig. 7(a), the lattice dimensionality D has the relative small effect on the effective mass when the interaction is small ($c=0.01$); however, the effective mass becomes sensitive to the dimensionality D with an increase of the interaction as shown in Fig. 7(b).

We have already mentioned that the analytical tight-binding result, Eq. (41), works only for the case of a weak interaction and large lattice potential and does not agree well with the numerical results in the case of a strong interaction.

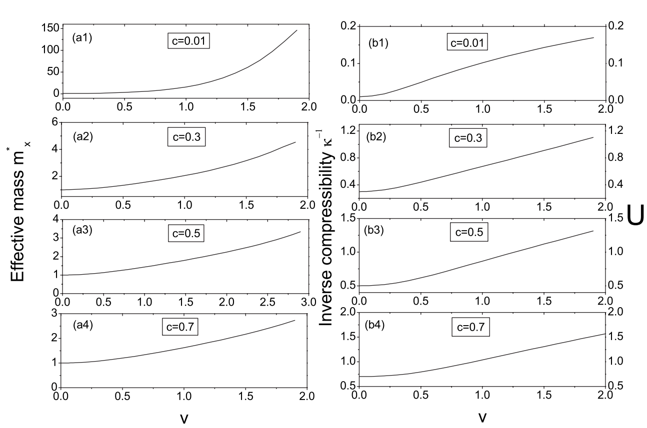

FIG. 6. Inverse compressibility κ^{-1} and effective mass m_x^* for a BEC in a 3D optical lattice via the strength of the optical lattice. Based on Eq. (38), U is equal to κ^{-1} in the tight-binding limit. The nonlinear coefficient $c=\pi n_0 a_s/k_L^2$, inverse compressibility κ^{-1} and U are in units of $4\hbar^2 k_L^2/m$, and the lattice strength of v is in units of $4\hbar^2 k_L^2/m$.

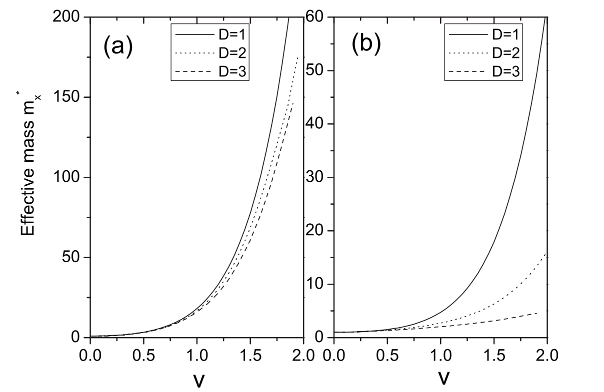

FIG. 7. Interplay between the effects of lattice dimensions and interactions on the effective mass: (a) $c=0.01$ and (b) $c=0.3$. The nonlinear coefficient $c=\pi n_0 a_s/k_L^2$ and the lattice strength of v is in units of $4\hbar^2 k_L^2/m$.

Here we explain it with the help of our numerical results of the tunneling rate J_x in Fig. 8, which is computed via Eq. (38). It is clear from Fig. 8 that the agreement between the tight-binding result, Eq. (40), and our numerical results gets worse from 1D to 3D. For example, at $v=1.5$, the agreement is quite good for $c=0.01, 0.2, 0.4$ in 1D while the agreement is only good for $c=0.01$ and $c=0.1$ in 2D and for $c=0.01$ in 3D. This shows that the interaction can affect J_x greatly in 2D and 3D. This influence is transferred to the sound speed via Eq. (37). This explains why the tight-binding result, Eq. (41), does not agree well with the numerical results in the case of strong interaction since the interaction is ignored in deriving Eq. (41).

We point out here that our study has been done with the Gross-Pitaevskii equation. In this mean-field theory, all

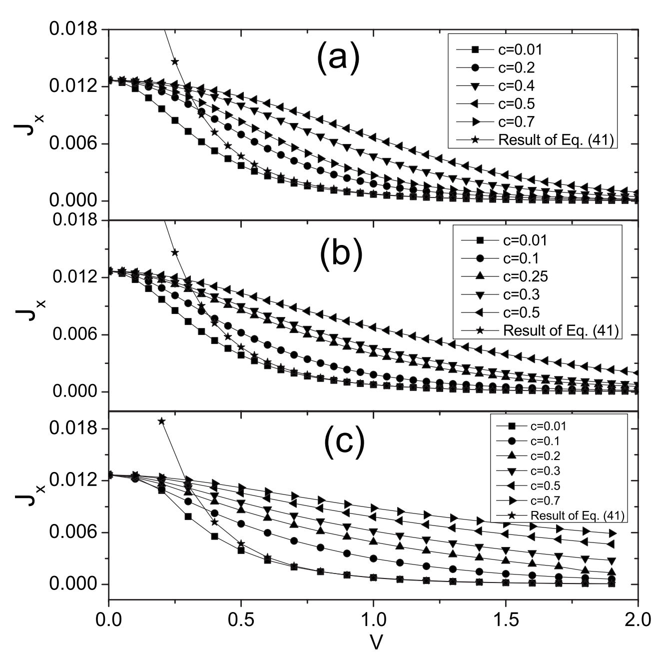

FIG. 8. Tunneling rate J_x via strength of optical lattice: (a) one-dimensional case, (b) two-dimensional case, and (c) three-dimensional case. The nonlinear coefficient $c=\pi n_0 a_s/k_L^2$, the tunneling rate J_x is in units of $4\hbar^2 k_L^2/m$, and the lattice strength of v is in units of $4\hbar^2 k_L^2/m$.

quantum fluctuations and temperature effects are ignored. To study the effects of temperature or fluctuations, in particular, near the transition point of superfluid and Mott insulator, one has to use other theories [40,41].

V. EXPERIMENTS

The speed of sound of a BEC in an optical lattice may be measured with a similar technique as was used in Ref. [13] to measure the sound speed of a BEC in a trap. Some complication is expected due to the periodic modulation of the BEC density. Another possible method is to employ Bragg spectroscopy [22,42,43] to the excitation spectrum. The speed of sound can be extracted from the slope of the linear part of the excitation spectrum.

In typical experiments to date, the relevant parameters are as follows: for a BEC in a three-dimensional optical lattice [11], the atom occupancy per lattice is of the order of $\langle n_i\rangle \approx 1-3$, $n_0=1.3-3.9\times 10^{19}$ m^{-3}, $k_L=2\pi/\lambda_L=7.37\times 10^6$ m^{-1}, and $a_s=5.4$ nm; for a BEC in a quasi-two-dimensional optical lattice [44], the atom occupancy per lattice can reach $\langle n_i\rangle \approx 170$, $n_0=3.6\times 10^{20}$ m^{-3}, $k_L=2\pi/\lambda_L=7.37\times 10^6$ m^{-1}, and $a_s=5.4$ nm; for a BEC in a quasi-one dimensional optical lattice [45], $\langle n_i\rangle \approx 1000$, $n_0=2.8\times 10^{20}$ m^{-3}, $k_L=2\pi/\lambda_L=7.9\times 10^6$ m^{-1}, and $a_s=5.4$ nm. These parameters correspond to $c=0.08$ for 1D optical lattices, $c=0.11$ for 2D optical lattices, and $c=0.004-0.012$ for 3D optical lattices. The depth of the optical lattice V_0 can be changed from $0E_R$ to $32E_R$ [11]; it means that our v can be changed from 0 and 2. To our knowledge, the highest atomic density without lattice is $n_0=3\times 10^{21}$ m^{-3} for sodium [46]. For this high density, we have $c=0.22$ with $k_L=1.07\times 10^7$ m^{-1} [4]. However, this is rather idealistic. The other possible way to increase c is to tune the scattering length a_s with Feshbach resonance [47,48].

VI. CONCLUSIONS

We have studied the speed of sound, compressibility, and effective mass of a Bose-Einstein condensate in an optical lattice both analytically and numerically. Special attention has been paid to the effect of the depth of the optical lattice, v; the interatomic interaction c; and the dimensionality D on the sound speed. Our investigation shows that the sound speed depends strongly on the strength of the lattice. In the one-dimensional case, the speed of sound falls monotonically with increasing lattice strength. The dependence becomes much richer in two and three dimensions. In the two-dimensional case, when the interaction is weak, the sound speed first increases and then decreases as the lattice strength increases. For the three-dimensional case, the sound speed can even oscillate with the lattice strength. These rich behaviors can be understood in terms of competition between compressibility and effective mass. Our analytical results at the limit of weak lattices also offer an interesting perspective to the understanding: they show that the lattice component perpendicular to the sound propagation decreases the sound speed while the lattice component parallel to the propagation increases the sound speed.

ACKNOWLEDGMENTS

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APPENDIX A: PRELIMINARY NOTATIONS

Suppose $f(\vec{r})$ to be a periodic function with periodicity of $\vec{R}$, given by

$$f(\vec{r}) = f(\vec{r}+\vec{R}), \tag{A1}$$

with

$$\vec{R} = m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3, \tag{A2}$$

where $\vec{r}$ is the position vector, $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ are any three vectors not all in the same plane, and m_1, m_2, and m_3 range through all integral values. Corresponding to $\vec{a}_i$'s, there exist a set of reciprocal vectors $\vec{b}_j$'s such that

$$\vec{a}_i\cdot\vec{b}_j = 2\pi\delta_{ij}. \tag{A3}$$

We can expand the periodic function $f(\vec{r})$ as its Fourier coefficients $\mathcal{F}_{\vec{n}}(f)$ as defined by

$$f(\vec{r}) = \sum_{\vec{n}} \mathcal{F}_{\vec{n}}(f)\exp\{i\vec{n}\cdot\vec{r}\}, \tag{A4}$$

with

$$\mathcal{F}_{\vec{n}}(V) = \frac{1}{\Omega}\int_{cell} d\vec{r}\, f(\vec{r})\exp\{-i\vec{n}\cdot\vec{r}\} \tag{A5}$$

and

$$\vec{n} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3, \tag{A6}$$

where the n_j are integers. In the integration, Ω is the volume of the primitive cell and the integration is over a primitive cell.

APPENDIX B: SOLUTIONS OF THE GROSS-PITAEVSKII EQUATION IN THE WEAK POTENTIAL LIMIT

The time-independent Gross-Pitaevskii (GP) equation in the three-dimensional case can be written as

$$-\frac{1}{2}\nabla^2\psi(\vec{r}) + c|\psi(\vec{r})|^2\psi(\vec{r}) + V_{ar}(\vec{r})\psi(\vec{r}) = \mu\psi(\vec{r}), \tag{B1}$$

where $V_{ar}(\vec{r})$ is the periodic potential with periodicity $\vec{R}$:

$$V_{ar}(\vec{r}) = V_{ar}(\vec{r}+\vec{R}). \tag{B2}$$

The Bloch-wave solution of the GP equation (B1) reads

$$\psi(\vec{r}) = \phi_{\vec{k}}(\vec{r})e^{i\vec{k}\cdot\vec{r}}, \tag{B3}$$

where $\vec{k}$ is the Bloch wave number and $\phi_{\vec{k}}(\vec{r})$ is a periodic function with the same periodicity of Eq. (B2). Substituting

Eq. (B3) into Eq. (B1), we have the following equation for each Bloch wave state $\phi_{\vec{k}}(\vec{r})$:

$$-\frac{1}{2}(\vec{\nabla}+i\vec{k})^2\phi_{\vec{k}}(\vec{r})+c|\phi_{\vec{k}}(\vec{r})|^2\phi_{\vec{k}}(\vec{r})+V_{ar}(\vec{r})\phi_{\vec{k}}(\vec{r})=\mu(\vec{k})\phi_{\vec{k}}(\vec{r}). \tag{B4}$$

The set of eigenvalues $\mu(\vec{k})$ then forms Bloch bands.

Besides the GP equation (B1), the Bloch wave function is also subject to the normalization condition given by

$$\frac{1}{\Omega}\int_{cell} d\vec{r}|\phi|^2=1, \tag{B5}$$

which is equivalent to

$$\mathcal{F}_{\vec{0}}(|\phi|^2)=1. \tag{B6}$$

For convenience, we have dropped the suffix $\vec{k}$ and the coordinate vector $\vec{r}$ in $\phi_{\vec{k}}(\vec{r})$.

Expanding ϕ in terms of the potential strength as

$$\phi=\phi^{(0)}+\phi^{(1)}+\phi^{(2)}+\cdots, \tag{B7}$$

we get the zeroth-, first-, and second-order forms of Eq. (B6), respectively:

$$\mathcal{F}_{\vec{0}}(|\phi|^2)^{(0)}=\sum_{\vec{n}}|\mathcal{F}_{\vec{n}}(\phi^{(0)})|^2=1, \tag{B8}$$

$$\mathcal{F}_{\vec{0}}(|\phi|^2)^{(1)}=\sum_{\vec{n}}[\mathcal{F}_{\vec{n}}(\phi^{(0)})\mathcal{F}^*_{\vec{n}}(\phi^{(1)})+\mathcal{F}_{\vec{n}}(\phi^{(1)})\mathcal{F}^*_{\vec{n}}(\phi^{(0)})]=0, \tag{B9}$$

$$\begin{aligned}\mathcal{F}_{\vec{0}}(|\phi|^2)^{(2)}=\sum_{\vec{n}}[&\mathcal{F}_{\vec{n}}(\phi^{(0)})\mathcal{F}^*_{\vec{n}}(\phi^{(2)})+|\mathcal{F}_{\vec{n}}(\phi^{(1)})|^2\\&+\mathcal{F}_{\vec{n}}(\phi^{(2)})\mathcal{F}^*_{\vec{n}}(\phi^{(0)})]=0.\end{aligned} \tag{B10}$$

There is still an arbitrary phase in the above wave functions, which satisfy both the GP equation and the normalization condition. Therefore, we may impose a third condition

$$\frac{1}{\Omega}\int d\vec{r}|\phi|^2\in\mathbb{R}, \tag{B11}$$

so that the Bloch states can be uniquely determined.

Before solving the GP equation (B1), we have to set forth another two specifications. First, we are only concerned with Bloch states at $\vec{k}=0$. In this case, we rewrite Eq. (B4) as follows:

$$-\frac{1}{2}\nabla^2\phi+c|\phi|^2\phi+V_{ar}(\vec{r})\phi=\mu\phi, \tag{B12}$$

where we dropped the suffix $\vec{0}$ and the coordinate vector $\vec{r}$ in $\phi_{\vec{0}}(\vec{r})$ for convenience. Expanding ϕ and μ in terms of the potential strength, we get the zeroth-, first-, and second-order forms of Eq. (B12), respectively:

$$-\frac{1}{2}\nabla^2\phi^{(0)}+c|\phi^{(0)}|^2\phi^{(0)}=\mu^{(0)}\phi^{(0)}, \tag{B13}$$

$$\begin{aligned}&-\frac{1}{2}\nabla^2\phi^{(1)}+c(2|\phi^{(0)}|^2\phi^{(1)}+\phi^{(0)^2}\phi^{(1)*})+V_{ar}(\vec{r})\phi^{(0)}\\&=\mu^{(0)}\phi^{(1)}+\mu^{(1)}\phi^{(0)},\end{aligned} \tag{B14}$$

$$\begin{aligned}&-\frac{1}{2}\nabla^2\phi^{(2)}+c(2|\phi^{(0)}|^2\phi^{(2)}+\phi^{(0)^2}\phi^{(2)*}+2\phi^{(0)}|\phi^{(1)}|^2\\&+\phi^{(0)*}\phi^{(1)^2})+V_{ar}(\vec{r})\phi^{(1)}=\mu^{(0)}\phi^{(2)}+\mu^{(1)}\phi^{(1)}+\mu^{(2)}\phi^{(0)}.\end{aligned} \tag{B15}$$

Second, we are only concerned with the cases in which the external potential $V_{ar}(\vec{r})$ is symmetric in each cell, or in other words, $V_{ar}(\vec{r})$ is an even function. Combining it with the condition that $V_{ar}(\vec{r})$ be a real function, we immediately have

$$\mathcal{F}_{\vec{n}}(V)=\mathcal{F}_{-\vec{n}}(V)\in\mathbb{R}. \tag{B16}$$

In the following, we will solve the GP equation for obtaining the normalized Bloch state at $\vec{k}=0$.

1. Zeroth-order correction of the GP equation

From Eq. (B13), we get the zeroth-order wave function and chemical potential, respectively,

$$\phi^{(0)}=1,\quad \mu^{(0)}=c, \tag{B17}$$

which automatically meet the normalization condition (B8).

2. First-order correction of the GP equation

Substituting Eq. (B17) into Eq. (B9), we have

$$\mathcal{F}_{\vec{0}}(\phi^{(1)})+\mathcal{F}^*_{\vec{0}}(\phi^{(1)})=0. \tag{B18}$$

From the phase condition (B11), we know that $\mathcal{F}_{\vec{0}}(\phi^{(1)})$ is a real number, and therefore

$$\mathcal{F}_{\vec{0}}(\phi^{(1)})=0. \tag{B19}$$

Substituting Eq. (B17) into Eq. (B14), we have

$$\frac{1}{2}|\vec{n}|^2\mathcal{F}_{\vec{n}}(\phi^{(1)})+c[\mathcal{F}_{\vec{n}}(\phi^{(1)})+\mathcal{F}_{\vec{n}}(\phi^{(1)*})]+\mathcal{F}_{\vec{n}}(V)=\mu^{(1)}\delta_{\vec{n}\cdot\vec{0}}. \tag{B20}$$

Plugging Eq. (B19) into Eq. (B20) and letting $\vec{n}=0$, we get the first-order correction of the chemical potential:

$$\mu^{(1)}=\mathcal{F}_{\vec{0}}(V). \tag{B21}$$

Taking complex conjugates on both sides of Eq. (B20) and replacing $-\vec{n}$ with $\vec{n}$, we obtain

$$\frac{1}{2}|\vec{n}|^2\mathcal{F}_{\vec{n}}(\phi^{(1)*})+c[\mathcal{F}_{\vec{n}}(\phi^{(1)})+\mathcal{F}_{\vec{n}}(\phi^{(1)*})]+\mathcal{F}_{\vec{n}}(V)=\mu^{(1)}\delta_{\vec{n}\cdot\vec{0}}. \tag{B22}$$

The unique solution of Eqs. (B20) and (B22) in the case of $\vec{n}\neq 0$ reads

$$\mathcal{F}_{\vec{n}}(\phi^{(1)})=\mathcal{F}_{\vec{n}}(\phi^{(1)*})=-\frac{\mathcal{F}_{\vec{n}}(V)}{\frac{1}{2}|\vec{n}|^2+2c},\quad \vec{n}\neq\vec{0}. \tag{B23}$$

From Eqs. (B19) and (B23), we know

$$\mathcal{F}_{\vec{n}}(\phi^{(1)})=\mathcal{F}_{-\vec{n}}(\phi^{(1)})\in\mathbb{R}, \tag{B24}$$

which means that $\phi^{(1)}(\vec{r})$ is a real even function.

3. Second-order correction of the GP equation

Plugging Eqs. (B17) and (B19) into Eq. (B10), we obtain

$$\mathcal{F}_{\vec{0}}(\phi^{(2)})+\mathcal{F}_{\vec{0}}(\phi^{(2)})^*+\sum_{\vec{n}}\mathcal{F}_{\vec{n}}(\phi^{(1)})^2=0. \tag{B25}$$

Plugging Eqs. (B17) and (B19) into Eq. (B15), we obtain

$$\frac{1}{2}|\vec{n}|^2\mathcal{F}_{\vec{n}}(\phi^{(2)})+c[\mathcal{F}_{\vec{n}}(\phi^{(2)})+\mathcal{F}_{\vec{n}}(\phi^{(2)^*})+3\mathcal{F}_{\vec{n}}(\phi^{(1)^2})]+\mathcal{F}_{\vec{n}}(V_{ar}\phi^{(1)})=\mu^{(1)}\mathcal{F}_{\vec{n}}(\phi^{(1)})+\mu^{(2)}\delta_{\vec{n}\cdot\vec{0}}. \tag{B26}$$

In the case of $\vec{n}=0$, we have

$$c[\mathcal{F}_{\vec{0}}(\phi^{(2)})+\mathcal{F}_{\vec{0}}(\phi^{(2)^*})+3\mathcal{F}_{\vec{0}}(\phi^{(1)^2})]+\mathcal{F}_{\vec{0}}(V\phi^{(1)})=\mu^{(1)}\mathcal{F}_{\vec{0}}(\phi^{(1)})+\mu^{(2)}\delta_{\vec{n}\cdot\vec{0}}. \tag{B27}$$

Plugging Eqs. (B21), (B23), and (B25) into Eq. (B27), we obtain the second-order correction of the chemical potential:

$$\mu^{(2)}=-\sum_{\vec{n}\neq\vec{0}}\frac{\frac{1}{2}|\vec{n}|^2}{\left(\frac{1}{2}|\vec{n}|^2+2c\right)^2}\mathcal{F}_{\vec{n}}(V)^2. \tag{B28}$$

To complete the calculation of the sound speed, we also need to calculate the system energy near $\vec{k}=0$. This can be obtained in terms of the effective potential $c|\phi|^2+V_{ar}(\vec{r})-\mu$ seen by each atom. We view our system as a noninteracting gas in the effective potential:

$$V_{eff}(\vec{r})=\frac{|\vec{n}|^2}{|\vec{n}|^2+4c}V(\vec{r}). \tag{B29}$$

Since the correction to the system energy is second order in the potential strength, it is sufficient to consider the first-order correction of the Bloch state; there is no need of calculating the second-order correction of the Bloch state. Based on Eq. (B29), we can easily obtain the system energy $E(\vec{k})$ near $\vec{k}=0$, up to the second-order correction:

$$E(\vec{k})=\frac{|\vec{k}|^2}{2}-\sum_{\vec{n}\neq 0}\frac{\frac{|\vec{n}|^4}{(|\vec{n}|^2+4c)^2}}{\frac{1}{2}(\vec{n}+\vec{k})^2-\frac{1}{2}|\vec{k}|^2}\mathcal{F}_{\vec{n}}^2(V). \tag{B30}$$

APPENDIX C: ANALYTICAL EXPRESSION OF SOUND SPEED BASED ON EQ. (17) IN THE WEAK POTENTIAL LIMIT

The aim of this section is to calculate the compressibility κ and the effective mass m^* as a function of the interatomic interaction c and of the depth of the arbitrary periodic potential $V_{ar}(\vec{r})$. Using these quantities, we will calculate the velocity of sound.

Compressibility κ and effective mass m^*

Plugging Eqs. (B17), (B21), and (B28) into Eq. (18), we obtain the analytical expression of compressibility κ in the weak potential limit:

$$\kappa^{-1}=c\left(1-\sum_{\vec{n}\neq 0}\frac{16|\vec{n}|^2}{(|\vec{n}|^2+4c)^3}\mathcal{F}_{\vec{n}}^2(V)\right). \tag{C1}$$

To calculate the sound speed, we also need calculating the effective mass m^*. Substituting Eq. (B30) into Eq. (6), we obtain the analytical expression of the effective mass along a given direction indicated by a unit vector $\hat{r}$:

$$\frac{1}{m^*}=1-\sum_{\vec{n}\neq 0}\frac{16|\vec{n}\cdot\hat{r}|^2}{|\vec{n}|^2(|\vec{n}|^2+4c)^2}\mathcal{F}_{\vec{n}}^2(V). \tag{C2}$$

We also find that the effective masses along each axis $\vec{x}$, $\vec{y}$, and $\vec{z}$ labeled by m_x^*, m_y^*, and m_z^* read

$$\frac{1}{m_x^*}=1-\sum_{\vec{n}\neq 0}\frac{16|\vec{n}\cdot\vec{x}|^2}{|\vec{n}|^2(|\vec{n}|^2+4c)^2}\mathcal{F}_{\vec{n}}^2(V), \tag{C3}$$

$$\frac{1}{m_y^*}=1-\sum_{\vec{n}\neq 0}\frac{16|\vec{n}\cdot\vec{y}|^2}{|\vec{n}|^2(|\vec{n}|^2+4c)^2}\mathcal{F}_{\vec{n}}^2(V), \tag{C4}$$

and

$$\frac{1}{m_z^*}=1-\sum_{\vec{n}\neq 0}\frac{16|\vec{n}\cdot\vec{z}|^2}{|\vec{n}|^2(|\vec{n}|^2+4c)^2}\mathcal{F}_{\vec{n}}^2(V). \tag{C5}$$

Plugging Eqs. (C2) and (C1) into Eq. (17), we arrive at the analytical expression of sound speed labeled by v_s along a given direction $\hat{r}$,

$$v_s=\sqrt{c}+8\sqrt{c}\left\{\sum_{\vec{n}\neq 0}\frac{|\vec{n}|^2}{(4c+|\vec{n}|^2)^3}-\sum_{\vec{n}\neq 0}\frac{|\vec{n}\cdot\hat{r}|^2}{|\vec{n}|^2(4c+|\vec{n}|^2)^2}\right\}\mathcal{F}_{\vec{n}}^2(V). \tag{C6}$$

Plugging Eqs. (C3)–(C5) and (C1), into Eq. (17), we also obtain the analytical expressions of sound speed along each axis $\vec{x}$, $\vec{y}$, and $\vec{z}$, labeled by v_{sx}, v_{sy}, and v_{sz}:

$$v_{s,x} = \sqrt{c} + 8\sqrt{c}\left\{\sum_{\vec{n}\neq 0}\frac{|\vec{n}|^2}{(4c+|\vec{n}|^2)^3} - \sum_{\vec{n}\neq 0}\frac{|\vec{n}\cdot\vec{x}|^2}{|\vec{n}|^2(4c+|\vec{n}|^2)^2}\right\}\mathcal{F}_{\vec{n}}^2(V), \tag{C7}$$

$$v_{s,y} = \sqrt{c} + 8\sqrt{c}\left\{\sum_{\vec{n}\neq 0}\frac{|\vec{n}|^2}{(4c+|\vec{n}|^2)^3} - \sum_{\vec{n}\neq 0}\frac{|\vec{n}\cdot\vec{y}|^2}{|\vec{n}|^2(4c+|\vec{n}|^2)^2}\right\}\mathcal{F}_{\vec{n}}^2(V), \tag{C8}$$

and

$$v_{s,z} = \sqrt{c} + 8\sqrt{c}\left\{\sum_{\vec{n}\neq 0}\frac{|\vec{n}|^2}{(4c+|\vec{n}|^2)^3} - \sum_{\vec{n}\neq 0}\frac{|\vec{n}\cdot\vec{z}|^2}{|\vec{n}|^2(4c+|\vec{n}|^2)^2}\right\}\mathcal{F}_{\vec{n}}^2(V). \tag{C9}$$

In the following, we consider a special case—i.e., where $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ are chosen along $\vec{x}$, $\vec{y}$, and $\vec{z}$, respectively; we also suppose $|\vec{a}_1|=|\vec{a}_2|=|\vec{a}_3|=2\pi$, without loss of generality. In this case, the sound speed of Eqs. (C7)–(C9) can be simplified into

$$v_{s,x} = \sqrt{c} + 8\sqrt{c}\left\{\sum_{\vec{n}\neq 0}\frac{\vec{n}^2}{(4c+\vec{n}^2)^3} - \sum_{\vec{n}\neq 0}\frac{n_1^2}{\vec{n}^2(4c+\vec{n}^2)^2}\right\}\mathcal{F}_{\vec{n}}^2(V), \tag{C10}$$

$$v_{s,y} = \sqrt{c} + 8\sqrt{c}\left\{\sum_{\vec{n}\neq 0}\frac{\vec{n}^2}{(4c+\vec{n}^2)^3} - \sum_{\vec{n}\neq 0}\frac{n_2^2}{\vec{n}^2(4c+\vec{n}^2)^2}\right\}\mathcal{F}_{\vec{n}}^2(V), \tag{C11}$$

and

$$v_{s,z} = \sqrt{c} + 8\sqrt{c}\left\{\sum_{\vec{n}\neq 0}\frac{\vec{n}^2}{(4c+\vec{n}^2)^3} - \sum_{\vec{n}\neq 0}\frac{n_3^2}{\vec{n}^2(4c+\vec{n}^2)^2}\right\}\mathcal{F}_{\vec{n}}^2(V). \tag{C12}$$

APPENDIX D: ANALYTICAL EXPRESSION OF SOUND SPEED BASED ON EQ. (16) IN THE WEAK POTENTIAL LIMIT

As shown in Sec. II B, there are two equivalent ways to calculate the velocity of sound; one is based on Eq. (16), and the other comes from Eq. (17). The aim of this section is to calculate the analytical expression of sound speed based on Eq. (16) from the another angle by directly solving excitation energy $\epsilon(q)$.

1. Matrices *P*, *Q*, *S*, and *T*

According to the Bogoliubov theory, the excitation energy $\epsilon(q)$ of the BEC in the Bloch state at $\vec{k}=0$ can be obtained by solving the eigenvalue problem

$$\delta_z M(\vec{q})\begin{pmatrix} u \\ v \end{pmatrix} = \epsilon(q)\begin{pmatrix} u \\ v \end{pmatrix}, \tag{D1}$$

with

$$M = \begin{pmatrix} \mathcal{L}(\vec{k}+\vec{q}) & c\phi_{\vec{k}}^2 \\ c\phi_{\vec{k}}^{*2} & \mathcal{L}(-\vec{k}+\vec{q}) \end{pmatrix} \tag{D2}$$

and

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{D3}$$

where $\mathcal{L}(\vec{p})$ is defined as

$$\mathcal{L}(\vec{q}) = -\frac{1}{2}(\vec{\nabla}+i\vec{q})^2 + V_{ar}(\vec{r}) - \mu + 2c|\phi_{\vec{k}}|^2. \tag{D4}$$

By a similarity transformation, we can transform $\sigma_z M$ into a numerical matrix P without changing the eigenvalues. The new matrix P can be represented in a block form

$$P = (T_{\vec{m}\cdot\vec{n}})_{\infty\times\infty}, \tag{D5}$$

where each block $T_{\vec{m}\cdot\vec{n}}$ is actual a 2×2 matrix and $\vec{m}$ and $\vec{n}$ take values ranging from $(-\infty,-\infty,-\infty)$ to $(+\infty,+\infty,+\infty)$. For convenience, we abbreviate the diagonal blocks $T_{\vec{n}\cdot\vec{n}\cdot}$ in Eq. (D5) as $S_{\vec{n}}$, and consequently $T_{\vec{m}\cdot\vec{n}}$ denotes solely those nondiagonal $(\vec{m}\neq\vec{n})$ blocks.

For we are only concerned with the case of $\vec{k}=0$, $\sigma_z M$ can be simplified into

$$\sigma_z M = \begin{pmatrix} \mathcal{L}(\vec{q}) & c\phi^2 \\ -c\phi^{*2} & -\mathcal{L}(\vec{q}) \end{pmatrix}. \tag{D6}$$

In this case, we have

$$S_{\vec{n}} = \begin{pmatrix} a_{\vec{n}} & b_{\vec{n}} \\ -b_{\vec{n}}^* & -a_{\vec{n}} \end{pmatrix}, \quad T_{\vec{m}\cdot\vec{n}} = \begin{pmatrix} c_{\vec{m}\cdot\vec{n}} & d_{\vec{m}\cdot\vec{n}} \\ -d_{\vec{m}\cdot\vec{n}}^* & -c_{\vec{m}\cdot\vec{n}} \end{pmatrix}, \tag{D7}$$

with $a_{\vec{n}}$, $b_{\vec{n}}$, $c_{\vec{m}\cdot\vec{n}}$ and $d_{\vec{m}\cdot\vec{n}}$ determined by

$$a_{\vec{n}} = \frac{1}{2}(\vec{n}+\vec{q})^2 + \mathcal{F}_0(V) - \mu + 2c\mathcal{F}_0(|\phi|^2), \tag{D8}$$

$$b_{\vec{n}} = c\mathcal{F}_0(\phi^2), \tag{D9}$$

$$c_{\vec{m}\cdot\vec{n}} = \mathcal{F}_{\vec{m}-\vec{n}}(V) + 2c\mathcal{F}_{\vec{m}-\vec{n}}(|\phi|^2), \tag{D10}$$

$$d_{\vec{m}\cdot\vec{n}} = c\mathcal{F}_{\vec{m}-\vec{n}}(\phi^2). \tag{D11}$$

We define the matrix Q as follows:

$$Q = P - \varepsilon I, \tag{D12}$$

where ε represents the lowest elementary excitation. Consequently, we have

$$\det Q = 0. \tag{D13}$$

Now, we compute the elements $a_{\vec{n}}$, $b_{\vec{n}}$, $c_{\vec{m}\cdot\vec{n}}$, and $d_{\vec{m}\cdot\vec{n}}$ from Eqs. (D8)–(D11) as follows:

$$a_{\vec{n}}^{(0)} = \frac{1}{2}(\vec{n}+\vec{q})^2 + c, \quad b_{\vec{n}}^{(0)} = c, \tag{D14}$$

$$c_{\vec{m}\cdot\vec{n}}^{(0)} = 0, \quad d_{\vec{m}\cdot\vec{n}}^{(0)} = 0, \tag{D15}$$

$$a_{\vec{n}}^{(1)} = 0, \quad b_{\vec{n}}^{(1)} = 0, \tag{D16}$$

$$c_{\vec{m}\cdot\vec{n}}^{(1)} = \frac{\frac{1}{2}(\vec{m}-\vec{n})^2 - 2c}{\frac{1}{2}(\vec{m}-\vec{n})^2 + 2c}\mathcal{F}_{\vec{m}-\vec{n}}(V), \tag{D17}$$

$$d_{\vec{m}\cdot\vec{n}}^{(1)} = -\frac{2c}{\frac{1}{2}(\vec{m}-\vec{n})^2 + 2c}\mathcal{F}_{\vec{m}-\vec{n}}(V), \tag{D18}$$

$$a_{\vec{n}}^{(2)} = \sum_{\vec{n}\neq\vec{0}} \frac{\frac{1}{2}\vec{n}^2}{\left(\frac{1}{2}\vec{n}^2 + 2c\right)^2}\mathcal{F}_{\vec{n}}(V)^2, \tag{D19}$$

$$b_{\vec{n}}^{(2)} = 0. \tag{D20}$$

For all these quantities real, we may drop the asterisks (*) in Eq. (D7).

2. Lowest elementary excitation in the weak potential limit

We expand the matrix Q and ε in terms of v as follows:

$$Q = Q^{(0)} + Q^{(1)} + Q^{(2)} + \cdots, \tag{D21}$$

$$\varepsilon = \varepsilon^{(0)} + \varepsilon^{(1)} + \varepsilon^{(2)} + \cdots. \tag{D22}$$

The aim of this subsection is to calculate $\varepsilon^{(0)}$, $\varepsilon^{(1)}$, and $\varepsilon^{(2)}$ by expanding Eq. (D13) into its zeroth-, first-, and second-order forms.

a. Zeroth-order approximation of ε

The zeroth-order form of Eq. (D13) is

$$(\det Q)^{(0)} = \det Q^{(0)} = \det(P^{(0)} - \varepsilon^{(0)}I) = 0. \tag{D23}$$

From Eqs. (D15), we know that all $T_{\vec{m}\cdot\vec{n}}^{(0)}$ are zero matrices, and therefore the matrix $P^{(0)}$ is block diagonal as represented in Eq. (D5). Consequently, the eigenvalues of $P^{(0)}$ are the collection of the eigenvalues of each $S_{\vec{n}}^{(0)}$. The zeroth-order approximation of ε is hence the positive eigenvalue of $S_{\vec{0}}^{(0)}$:

$$\begin{vmatrix} a_{\vec{0}}^{(0)} - \varepsilon^{(0)} & b_{\vec{0}}^{(0)} \\ -b_{\vec{0}}^{(0)} & -a_{\vec{0}}^{(0)} - \varepsilon^{(0)} \end{vmatrix} = 0. \tag{D24}$$

The positive solution of Eq. (D24) reads

$$\varepsilon^{(0)} = \sqrt{\frac{1}{4}\vec{q}^4 + c\vec{q}^2}. \tag{D25}$$

With the value of $\varepsilon^{(0)}$, we calculate the determinant of each diagonal block of the matrix $Q^{(0)}$:

$$\det(S_{\vec{n}}^{(0)} - \varepsilon^{(0)}I) = \left(\frac{1}{2}\vec{q}^2 + c\right)^2 - \left(\frac{1}{2}(\vec{n}+\vec{q})^2 + c\right)^2, \tag{D26}$$

which are denoted by $\mathcal{R}_{\vec{n}}$ for convenience,

$$\mathcal{R}_{\vec{n}} = \left(\frac{1}{2}\vec{q}^2 + c\right)^2 - \left(\frac{1}{2}(\vec{n}+\vec{q})^2 + c\right)^2. \tag{D27}$$

This result will be useful in the following sections.

b. First-order correction of ε

We can conclude that the first-order correction of ε vanishes as

$$\varepsilon^{(1)} = 0. \tag{D28}$$

c. Second-order correction of ε

The second-order form of Eq. (D13) reads

$$(\det Q)^{(2)} = \sum_{ij}\left(\frac{\partial|Q|}{\partial Q_{ij}}\right)^{(0)} Q_{ij}^{(2)} + \frac{1}{2}\sum_{ijkl}\left(\frac{\partial^2|Q|}{\partial Q_{ij}\partial Q_{kl}}\right)^{(0)} Q_{ij}^{(1)}Q_{kl}^{(1)} = 0. \tag{D29}$$

Here we introduce the "second cofactor matrix" of Q, which is denoted by $\tilde{\tilde{Q}}$ and whose elements are defined as

$$\tilde{\tilde{Q}}_{ij,kl} = \frac{\partial^2|Q|}{\partial Q_{ij}\partial Q_{kl}}. \tag{D30}$$

By this notation, we reduce Eq. (D29) to

$$\sum_{ij}\tilde{Q}_{ij}^{(0)}Q_{ij}^{(2)} + \frac{1}{2}\sum_{ijkl}\tilde{\tilde{Q}}_{ij,kl}^{(0)}Q_{ij}^{(1)}Q_{kl}^{(1)} = 0. \tag{D31}$$

We start by computing the first term on the left-hand side of Eq. (D31). Keeping only the nonvanishing terms and noting that $\mathcal{R}_{\vec{0}}=0$, we have

$$\sum_{ij}\tilde{Q}_{ij}^{(0)}Q_{ij}^{(2)} = \sum_{\vec{n}}(2\varepsilon^{(0)}\varepsilon^{(2)} - 2a_{\vec{n}}^{(0)}a_{\vec{n}}^{(2)})\prod_{\vec{m}\neq\vec{n}}\mathcal{R}_{\vec{m}} = (2\varepsilon^{(0)}\varepsilon^{(2)} - 2a_{\vec{0}}^{(0)}a_{\vec{0}}^{(2)})\prod_{\vec{m}\neq\vec{0}}\mathcal{R}_{\vec{m}}. \tag{D32}$$

Then we proceed to compute the second term on the left-hand side of Eq. (D31). It should be noted that any Q_{ij} is one of the elements of the matrix $U_{\vec{m}\cdot\vec{n}}$, which is defined as

$$U_{\vec{m}\cdot\vec{n}} = \begin{pmatrix} a_{\vec{m}} - \varepsilon & b_{\vec{m}} & c_{\vec{m}\cdot\vec{n}} & d_{\vec{m}\cdot\vec{n}} \\ -b_{\vec{m}} & -a_{\vec{m}} - \varepsilon & -d_{\vec{m}\cdot\vec{n}} & -c_{\vec{m}\cdot\vec{n}} \\ c_{\vec{n}\cdot\vec{m}} & d_{\vec{n}\cdot\vec{m}} & a_{\vec{n}} - \varepsilon & b_{\vec{n}} \\ -d_{\vec{n}\cdot\vec{m}} & -c_{\vec{n}\cdot\vec{m}} & -b_{\vec{n}} & -a_{\vec{n}} - \varepsilon \end{pmatrix}. \tag{D33}$$

The second term on the left-hand side of Eq. (D31) could be computed in a routine way by computing the second cofactor matrix of $U_{\vec{m}\cdot\vec{n}}$. However, we have found a much more convenient method to compute this term which is shown as follows. Since we have

$$a_{\vec{m}}^{(1)} - \varepsilon^{(1)} = - a_{\vec{m}}^{(1)} - \varepsilon^{(1)} = b_{\vec{m}}^{(1)} = - b_{\vec{m}}^{(1)} = 0, \tag{D34}$$

the only nonvanishing $Q_{ij}^{(1)}$ are those in $T_{\vec{m}\cdot\vec{n}}^{(1)}$, or more specifically, $c_{\vec{m}\cdot\vec{n}}^{(1)}$, $-c_{\vec{m}\cdot\vec{n}}^{(1)}$, $d_{\vec{m}\cdot\vec{n}}^{(1)}$, and $-d_{\vec{m}\cdot\vec{n}}^{(1)}$. We further assert that in order to get a nonvanishing $\tilde{\tilde{Q}}_{ij,kl}^{(0)}$, the corresponding Q_{ij} and Q_{kl} must be in the same $U_{\vec{m}\cdot\vec{n}}$. This assertion can be confirmed by some routine proof which we shall not elaborate here. From the above assertion, we obtain the expression

$$\sum_{ijkl} \tilde{\tilde{Q}}_{ij,kl}^{(0)} Q_{ij}^{(1)} Q_{kl}^{(1)} = \sum_{\vec{m},\vec{n}}^{\vec{m}\neq\vec{n}} \sum_{ijkl=1}^{4} (\tilde{\tilde{U}}_{\vec{m}\cdot\vec{n}})_{ij,kl}^{(0)} (U_{\vec{m}\cdot\vec{n}})_{ij}^{(1)} \times (U_{\vec{m}\cdot\vec{n}})_{kl}^{(1)} \prod_{\vec{k}\neq\vec{m},\vec{n}} \mathcal{R}_{\vec{k}}. \tag{D35}$$

Keeping only the second-order correction terms, we have

$$\begin{aligned}\sum_{ijkl=1}^{4} (\tilde{\tilde{U}}_{\vec{m}\cdot\vec{n}})_{ij,kl}^{(0)} (U_{\vec{m}\cdot\vec{n}})_{ij}^{(1)} (U_{\vec{m}\cdot\vec{n}})_{kl}^{(1)} &= - 2\varepsilon^{(0)^2} c_{\vec{m}\cdot\vec{n}}^{(1)} c_{\vec{n}\cdot\vec{m}}^{(1)} - 2a_{\vec{m}}^{(0)} a_{\vec{n}}^{(0)} c_{\vec{m}\cdot\vec{n}}^{(1)} c_{\vec{n}\cdot\vec{m}}^{(1)} - 2b_{\vec{m}}^{(0)} b_{\vec{n}}^{(0)} c_{\vec{m}\cdot\vec{n}}^{(1)} c_{\vec{n}\cdot\vec{m}}^{(1)} \\ &\quad + 2a_{\vec{n}}^{(0)} b_{\vec{m}}^{(0)} c_{\vec{n}\cdot\vec{m}}^{(1)} d_{\vec{m}\cdot\vec{n}}^{(1)} + 2a_{\vec{m}}^{(0)} b_{\vec{n}}^{(0)} c_{\vec{n}\cdot\vec{m}}^{(1)} d_{\vec{m}\cdot\vec{n}}^{(1)} \\ &\quad + 2a_{\vec{n}}^{(0)} b_{\vec{m}}^{(0)} c_{\vec{m}\cdot\vec{n}}^{(1)} d_{\vec{n}\cdot\vec{m}}^{(1)} + 2a_{\vec{m}}^{(0)} b_{\vec{n}}^{(0)} c_{\vec{m}\cdot\vec{n}}^{(1)} d_{\vec{n}\cdot\vec{m}}^{(1)} + 2\varepsilon^{(0)^2} d_{\vec{m}\cdot\vec{n}}^{(1)} d_{\vec{n}\cdot\vec{m}}^{(1)} \\ &\quad - 2a_{\vec{m}}^{(0)} a_{\vec{n}}^{(0)} d_{\vec{m}\cdot\vec{n}}^{(1)} d_{\vec{n}\cdot\vec{m}}^{(1)} - 2b_{\vec{m}}^{(0)} b_{\vec{n}}^{(0)} d_{\vec{m}\cdot\vec{n}}^{(1)} d_{\vec{n}\cdot\vec{m}}^{(1)},\end{aligned} \tag{D36}$$

which is denoted by $\mathcal{W}_{\vec{m}\cdot\vec{n}}$ for convenience. Since both $c_{\vec{m}\cdot\vec{n}}^{(1)}$ and $d_{\vec{m}\cdot\vec{n}}^{(1)}$ are symmetric in $\vec{m}$ and $\vec{n}$, the same is true for $\mathcal{W}_{\vec{m}\cdot\vec{n}}$:

$$\mathcal{W}_{\vec{m}\cdot\vec{n}} = \mathcal{W}_{\vec{n}\cdot\vec{m}}. \tag{D37}$$

Plugging Eq. (D36) into Eq. (D35) and noting that $\mathcal{R}_{\vec{0}} = 0$, we obtain

$$\sum_{ijkl} \tilde{\tilde{Q}}_{ij,kl}^{(0)} Q_{ij}^{(1)} Q_{kl}^{(1)} = 2 \sum_{\vec{n}\neq\vec{0}} \frac{\mathcal{W}_{\vec{n}\cdot\vec{0}}}{\mathcal{R}_{\vec{n}}} \prod_{\vec{m}\neq\vec{0}} \mathcal{R}_{\vec{n}}. \tag{D38}$$

Plugging Eqs. (D32) and (D38) into Eq. (D31), we have

$$(2\varepsilon^{(0)}\varepsilon^{(2)} - 2a_0^{(0)} a_0^{(2)}) \prod_{\vec{m}\neq\vec{0}} \mathcal{R}_{\vec{m}} + \sum_{\vec{n}\neq\vec{0}} \frac{\mathcal{W}_{\vec{n}\cdot\vec{0}}}{\mathcal{R}_{\vec{n}}} \prod_{\vec{m}\neq\vec{0}} \mathcal{R}_{\vec{m}} = 0, \tag{D39}$$

from which we finally arrive at the value of $\varepsilon^{(2)}$:

$$\varepsilon^{(2)} = \frac{1}{\varepsilon^{(0)}} \sum_{\vec{n}\neq\vec{0}} \left(a_0^{(0)} \frac{\frac{1}{2}|\vec{n}|^2}{\left(\frac{1}{2}|\vec{n}|^2 + 2c\right)^2} \mathcal{F}_{\vec{n}}(V)^2 - \frac{1}{2} \frac{\mathcal{W}_{\vec{n}\cdot\vec{0}}}{\mathcal{R}_{\vec{n}}} \right). \tag{D40}$$

3. Speed of sound in the weak potential limit

The speed of sound along any given direction $\hat{r}$ in a BEC is defined as

$$v_{\hat{n}} = |\vec{\nabla}_{\vec{q}} \varepsilon(\vec{q})|_{\vec{q}\to\vec{0}^+}. \tag{D41}$$

Let us consider a special case—i.e., where $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ are chosen along each axis of reference system, $\vec{x}$, $\vec{y}$, and $\vec{z}$, respectively; and without loss of generality, we suppose the periodicity of the periodic potential along each axis to be 2π. We are particularly interested in the speed of sound along one of the three axes—for example, the x-axis:

$$m_{s,x} = \left.\frac{\partial \varepsilon}{\partial q_x}\right|_{\vec{q}\to\vec{0}^+}. \tag{D42}$$

Plugging Eqs. (D25), (D28), and (D40), into Eq. (D42), we finally obtain the analytical expression of the sound speed along each axis:

$$v_{s,x} = \sqrt{c} + \sum_{\vec{n}\neq 0} \frac{8\sqrt{c}[(n_2^2 + n_3^2)|\vec{n}|^2 - 4cn_1^2]}{|\vec{n}|^2(4c + |\vec{n}|^2)^3} \mathcal{F}_{\vec{n}}^2(V), \tag{D43}$$

$$v_{s,y} = \sqrt{c} + \sum_{\vec{n}\neq 0} \frac{8\sqrt{c}[(n_1^2 + n_3^2)|\vec{n}|^2 - 4cn_2^2]}{|\vec{n}|^2(4c + |\vec{n}|^2)^3} \mathcal{F}_{\vec{n}}^2(V), \tag{D44}$$

and

$$v_{s,z} = \sqrt{c} + \sum_{\vec{n}\neq 0} \frac{8\sqrt{c}[(n_1^2 + n_2^2)|\vec{n}|^2 - 4cn_3^2]}{|\vec{n}|^2(4c + |\vec{n}|^2)^3} \mathcal{F}_{\vec{n}}^2(V). \tag{D45}$$

It can be easily proved that Eqs. (D43)–(D45) can be deduced from Eqs. (C10)–(C12).

APPENDIX E: A SPECIAL EXAMPLE

Suppose that the arbitrary potential of $V_{ar}(\vec{r})$ is chosen to be the special form of Eq. (2):

$$V_{latt}(\vec{r}) = v(\cos x + \cos y + \cos z). \tag{E1}$$

In this case, there are only six nonvanishing Fourier coefficients

$$\mathcal{F}_{\vec{n}}(V) = \frac{v}{2}(\delta_{\vec{n},(\pm 1,0,0)} + \delta_{\vec{n},(0,\pm 1,0)} + \delta_{\vec{n},(0,0,\pm 1)}). \tag{E2}$$

Submitting Eq. (E2) into Eq. (D43), we have

$$v_{s,x} = \sqrt{c}\left(1 + \frac{8(1-2c)}{(4c+1)^3} v^2\right), \quad \text{for } D = 3. \tag{E3}$$

With similar calculations, we can also obtain the analytic expressions of sound speed in the optical lattices of Eqs. (7) and (8), respectively:

$$v_{s,i} = \sqrt{c}\left(1 + \frac{16c}{(4c+1)^3}v^2\right), \quad \text{for } D = 1, \tag{E4}$$

$$v_{s,i} = \sqrt{c}\left(1 + \frac{8(1-4c)}{(4c+1)^3}v^2\right), \quad \text{for } D = 2, \tag{E5}$$

with $i = x, y, x$. Combining Eqs. (E3), (E5), and (E5) together, we arrive at

$$v_{s,i} = \sqrt{c}\left(1 + \frac{4(D-1-4c)}{(4c+1)^3}v^2\right), \quad i = x, y, z. \tag{E6}$$

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