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Angaben zur Veröffentlichung / Publication details:

Yukalov, Vyacheslav I., and Klaus G. Ziegler. 2015. "Instability of insulating states in optical lattices due to collective phonon excitations." *Physical Review A* 91 (2): 023628. https://doi.org/10.1103/physreva.91.023628.

Instability of insulating states in optical lattices due to collective phonon excitations

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(Received 23 July 2014; revised manuscript received 7 January 2015; published 25 February 2015)

The effect of collective phonon excitations on the properties of cold atoms in optical lattices is investigated. These phonon excitations are collective excitations, whose appearance is caused by intersite atomic interactions correlating the atoms, and they do not arise without such interactions. These collective excitations should not be confused with lattice vibrations produced by an external force. No such force is assumed. But the considered phonons are purely self-organized collective excitations, characterizing atomic oscillations around lattice sites, due to intersite atomic interactions. It is shown that these excitations can essentially influence the possibility of atoms' being localized. The states that would be insulating in the absence of phonon excitations can become delocalized when these excitations are taken into account. This concerns long-range as well as local atomic interactions. To characterize the region of stability, the Lindemann criterion is used.

DOI: 10.1103/PhysRevA.91.023628 PACS number(s): 67.85.Hj, 05.30.Jp, 67.80.de, 64.60.De

I. INTRODUCTION

Cold atoms in optical lattices are usually considered in the frame of the Hubbard model (see, e.g., reviews in [1–4]). The periodic potential of an optical lattice is imposed by external laser beams. This potential is fixed in space, prescribing a lattice formed by the lattice sites $\mathbf{a}_i$. We do not assume the existence of external fields that would move the lattice.

If atomic interactions between sites are neglected, the individual properties of atoms in each potential well are completely prescribed by the given optical lattice. However, as soon as the intersite atomic interactions are taken into account, the low-energy positions of the atoms are not exactly those of the potential minima of the optical lattice. In other words, an atom in a potential well experiences an oscillational motion due to the interaction with the other atoms. These oscillations, due to the interaction effect, can be characterized as collective phonon excitations.

It is these collective excitations that are considered in our paper. As is well known, collective excitations in many cases can essentially influence the system stability. Our aim is to study the role of such phonon excitations for atoms in optical lattices. We use the standard method of taking into account collective excitations, by considering small deviations from equilibrium values.

It is important to stress the necessity of intersite atomic interactions, without which phonon excitations cannot exist. The situations of externally shaking the lattice and of the existence of self-organized collective excitations in a system of correlated atoms are principally different and should not be confused. In the former case, vibrations should be produced by an external field and would exist without any intersite atomic interactions. But in the latter case, there is no external shaking field and the collective excitations do not exist in the absence of intersite atomic interactions.

It is the aim of the present paper to study the properties of insulating atomic states in optical lattices, taking into account the arising phonon excitations and their influence on the stability of the insulating states.

It turns out that phonon excitations can essentially influence the properties of atomic states in optical lattices. Such excitations play an important role in defining the boundary of the region where atoms can be localized. The presence of phonons can provoke an instability of an insulating state, triggering atomic delocalization, often destroying the insulating state that would exist without these excitations. This delocalization effect can occur for both types of atomic interactions, long-range as well as local.

Throughout the paper, the system of units is employed, where the Planck and Boltzmann constants equal to 1 ($\hbar = 1$, $k_B = 1$).

II. MAIN DEFINITIONS AND NOTATIONS

In this section, we give the main definitions and notations that are used in the following sections. We consider a fixed optical lattice described by the spatial points $\{\mathbf{a}_i\}$ corresponding to N_L lattice sites enumerated by the index $i = 1,2,\ldots,N_L$. The elementary lattice cell is characterized by the set of vectors $\mathbf{a} = \{a_\alpha\}$, where the spatial components are enumerated by the index $\alpha = 1,2,\ldots,d$. For the sake of generality, we consider a d-dimensional space, which makes it straightforward to analyze the particular cases of one-, two-, and three-dimensional lattices.

The lattice contains N atoms, whose ratio to the number of sites N_L defines the filling factor

$$\nu \equiv \frac{N}{N_L} = \rho a^d, \tag{1}$$

in which ρ is the average atomic density and a is the mean interatomic distance, given by the expressions

$$\rho \equiv \frac{N}{V}, \quad a \equiv \left(\frac{V}{N_L}\right)^{1/d}, \tag{2}$$

with V being the system volume. The filling factor can be an arbitrary positive number.

The optical lattice, formed by laser beams, is characterized by the lattice potential

$$V_L(\mathbf{r}) = \sum_{\alpha=1}^{d} V_\alpha \sin^2\left(k_0^\alpha r_\alpha\right), \tag{3}$$

where $k_0^\alpha = \pi/a_\alpha$. The recoil energy, playing the role of a characteristic kinetic energy, is denoted as

$$E_R = \frac{k_0^2}{2m} \quad \left(k_0^2 \equiv \frac{1}{d} \sum_{\alpha=1}^{d} \frac{\pi^2}{a_\alpha^2} \right), \tag{4}$$

with m being atomic mass. The Schrödinger lattice Hamiltonian is

$$H_L(\mathbf{r}) = -\frac{\nabla^2}{2m} + V_L(\mathbf{r}), \tag{5}$$

with the lattice potential, (3).

The extended Hubbard Hamiltonian is derived in the usual way. One starts with the standard Hamiltonian of atoms with pair interactions $\Phi(\mathbf{r})$, expands the field operators over the Wannier functions $w(\mathbf{r} - \mathbf{a}_i)$, and restricts the consideration to the lowest energy band. In what follows, we need the notations for the matrix elements over the Wannier functions: the hopping term

$$J_{ij} \equiv -\int w^*(\mathbf{r} - \mathbf{a}_i) H_L(\mathbf{r}) w(\mathbf{r} - \mathbf{a}_j) d\mathbf{r}, \tag{6}$$

the intersite interaction

$$U_{ij} \equiv \int |w(\mathbf{r} - \mathbf{a}_i)|^2 \Phi(\mathbf{r} - \mathbf{r}') |w(\mathbf{r}' - \mathbf{a}_j)|^2 d\mathbf{r} d\mathbf{r}', \tag{7}$$

the momentum squared

$$\mathbf{p}_j^2 \equiv \int w^*(\mathbf{r} - \mathbf{a}_j)(-\nabla^2) w(\mathbf{r} - \mathbf{a}_j) d\mathbf{r}, \tag{8}$$

and the average lattice parameter

$$V_L \equiv \int w^*(\mathbf{r}) V_L(\mathbf{r}) w(\mathbf{r}) d\mathbf{r}. \tag{9}$$

With these notations, one obtains the extended Hubbard Hamiltonian

$$\hat{H} = -\sum_{i \neq j} J_{ij} c_i^\dagger c_j + \sum_j \left(\frac{\mathbf{p}_j^2}{2m} + V_L \right) c_j^\dagger c_j + \frac{U}{2} \sum_j c_j^\dagger c_j^\dagger c_j c_j + \frac{1}{2} \sum_{i \neq j} U_{ij} c_i^\dagger c_j^\dagger c_j c_i, \tag{10}$$

in which $U \equiv U_{jj}$. The constant term V_L in Hamiltonian (10) can be omitted. In the hopping term, it is customary to consider only the nearest neighbors, denoting as J the value of J_{ij} related to these nearest neighbors. Neglecting the last term in Eq. (10), describing intersite atomic interactions, would reduce the Hamiltonian to the standard Hubbard model. This omission can be motivated by the fact that usually the value of U_{ij} for $i \neq j$ is smaller than the on-site interaction U. However, for the treatment of phonon excitations, the intersite interactions are crucial, even when they are small.

The atomic interactions, generally, contain two parts,

$$\Phi(\mathbf{r}) = \Phi_{\rm loc}(\mathbf{r}) + \Phi_{\rm non}(\mathbf{r}), \tag{11}$$

the local interactions, described by a δ function,

$$\Phi_{\rm loc}(\mathbf{r}) = \Phi_d \delta(\mathbf{r}), \tag{12}$$

and nonlocal long-range interactions $\Phi_{\rm non}(\mathbf{r})$, such as dipolar interactions [5–8]. The parameters of the local and nonlocal interactions can be connected, but to a large extent, the two types of the interactions can be treated as independent. Moreover, the strengths of these interactions can be varied over a wide range. Respectively, the interaction term, (7), is the sum of two parts,

$$U_{ij} = U_{ij}^{\rm loc} + U_{ij}^{\rm non}, \tag{13}$$

corresponding to local interactions,

$$U_{ij}^{\rm loc} = \Phi_d \int |w(\mathbf{r} - \mathbf{a}_i)|^2 |w(\mathbf{r} - \mathbf{a}_j)|^2 d\mathbf{r}, \tag{14}$$

and to nonlocal interactions,

$$U_{ij}^{\rm non} = \int |w(\mathbf{r} - \mathbf{a}_i)|^2 \Phi_{\rm non}(\mathbf{r} - \mathbf{r}') |w(\mathbf{r}' - \mathbf{a}_j)|^2 d\mathbf{r} d\mathbf{r}'. \tag{15}$$

The strength of the local interaction potential Φ_d depends on the system dimensionality and setup geometry. Considering a system with atomic dynamics in d dimensions, we can keep in mind the realistic situation, when $3 - d$ directions are confined to the ground state of a harmonic oscillator, with a frequency $\omega_\perp$, to a size $l_\perp \equiv 1/\sqrt{m\omega_\perp}$. Then we will have quasi-one-dimensional or quasi-two-dimensional systems [9,10].

For example, in three dimensions, the local-potential strength is

$$\Phi_3 \equiv \Phi_0 = 4\pi \frac{a_s}{m},$$

where a_s is the s-wave scattering length. For quasi-two-dimensional bosons [11], one has

$$\Phi_2 \cong \frac{\Phi_0}{\sqrt{2\pi}\, l_\perp - a_s \ln[(2\pi)^{3/2} \rho l_\perp a_s]}.$$

And for quasi-one-dimensional bosons [12], one gets

$$\Phi_1 \cong \frac{\Phi_0}{2\pi l_\perp (l_\perp - 0.46 a_s)}.$$

If the scattering length is much shorter than the length of the transverse confinement, then the above equations reduce to the formula

$$\Phi_d = \frac{\Phi_0}{(\sqrt{2\pi}\, l_\perp)^{3-d}} \quad \left(\frac{a_s}{l_\perp} \ll 1 \right).$$

All the cases considered above can be summarized in the form

$$\Phi_d = \frac{\Phi_{\rm eff}}{(\sqrt{2\pi}\, l_\perp)^{3-d}}, \tag{16}$$

in which the effective strength

$$\Phi_{\rm eff} = 4\pi \frac{a_{\rm eff}}{m} \tag{17}$$

is expressed through the effective scattering length. The latter in the quasi-one-dimensional case reads as

$$a_{\rm eff} = \frac{a_s}{1 - 0.46 a_s / l_\perp} \quad (d = 1); \tag{18}$$

in the quasi-two-dimensional case, it is

$$a_{\rm eff} = \frac{a_s}{1 - (a_s/\sqrt{2\pi}\, l_\perp) \ln[(2\pi)^{3/2} \rho l_\perp a_s]} \quad (d = 2); \tag{19}$$

and in three dimensions, it reduces to

$$a_{\rm eff} = a_s \quad (d = 3). \tag{20}$$

Above, we have listed the expressions that we need in what follows. The derivation of these formulas can be found in the cited literature. Typical expressions for the system parameters for an insulating state, such as the hopping term and intersite interactions, are given in Appendix A.

III. VIBRATIONAL COLLECTIVE EXCITATIONS

As is well known, collective excitations can essentially influence the system properties, defining the stability boundaries of different physical states [13]. Thus, the stability of an insulating state can depend on the existence of phonon excitations. These collective excitations can modify the properties of many-body systems, even when particle interactions are rather small. In particular, phonon excitations can destabilize the system, leading to particle delocalization destroying an insulating state. As examples of systems where phonon excitations can strongly influence the region of stability, we can mention ferroelectrics [14,15] and atoms in double-well potentials [16,17]. Here, we consider the effect of phonons on the stability of insulating states in optical lattices. Here and in what follows, speaking about insulating states, we keep in mind the states typical of Mott insulators. In such states, atoms are well localized. But the notion of localization is more general and essentially depends on atomic interactions. We employ the term "localization" in this general sense.

Collective excitations are usually introduced by considering small deviations from equilibrium values. Taking account of phonon excitations can be done in the traditional way [18,19] by considering vibrating atoms characterized by vectors $\mathbf{r}_j$, oscillating around the related lattice sites $\mathbf{a}_j$, and introducing the deviations $\mathbf{u}_j$ according to the rule

$$\mathbf{r}_j = \mathbf{a}_j + \mathbf{u}_j, \tag{21}$$

requiring the validity of the conditions for the averages

$$\mathbf{a}_j \equiv \langle \mathbf{r}_j \rangle, \quad \langle \mathbf{u}_j \rangle = 0, \tag{22}$$

where $\langle \cdots \rangle = {\rm Tr}[\cdots e^{-\beta H}]/{\rm Tr}[e^{-\beta H}]$ is an average with respect to the total Hamiltonian including all thermal and quantum fluctuations. A vanishing average $\mathbf{u}_j$ is based on the condition that the system is in stable equilibrium, where $\mathbf{a}_j$ is the definition of the lattice vectors prescribed by the given equilibrium optical lattice. The deviation $\mathbf{u}_j$ can become nonzero at points of instability, such as the Peierls instability.

The quantities $U(\mathbf{r}_{ij})$ and $J(\mathbf{r}_{ij})$ depend on the difference of the spatial variables

$$\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j = \mathbf{a}_{ij} + \mathbf{u}_{ij}, \tag{23}$$

where we use the notation

$$\mathbf{u}_{ij} \equiv \mathbf{u}_i - \mathbf{u}_j, \quad \mathbf{a}_{ij} = \mathbf{a}_i - \mathbf{a}_j. \tag{24}$$

It is worth mentioning the main difference between the optical lattice, whose periodicity and lattice vectors $\mathbf{a}_i$ are strictly prescribed by the imposed laser beams, and a self-organized crystal, whose lattice vectors $\mathbf{a}_i$ are defined self-consistently through the minimization of a thermodynamic potential.

In a localized state, atomic deviations from the lattice sites are supposed to be small, which justifies the expansion of the interaction potentials in powers of the deviations. As usual, restricting such an expansion by the second order, we have

$$\begin{aligned} U(\mathbf{r}_{ij}) &\simeq U_{ij} + \sum_\alpha U_{ij}^\alpha u_{ij}^\alpha - \frac{1}{2}\sum_{\alpha\beta} U_{ij}^{\alpha\beta} u_{ij}^\alpha u_{ij}^\beta, \\ J(\mathbf{r}_{ij}) &\simeq J_{ij} + \sum_\alpha J_{ij}^\alpha u_{ij}^\alpha - \frac{1}{2}\sum_{\alpha\beta} J_{ij}^{\alpha\beta} u_{ij}^\alpha u_{ij}^\beta, \end{aligned} \tag{25}$$

where we use the notations

$$\begin{aligned} &U_{ij} \equiv U(\mathbf{a}_{ij}), \quad J_{ij} \equiv J(\mathbf{a}_{ij}), \\ &U_{ij}^\alpha \equiv \frac{\partial U_{ij}}{\partial a_i^\alpha}, \quad J_{ij}^\alpha \equiv \frac{\partial J_{ij}}{\partial a_i^\alpha}, \quad U_{ij}^{\alpha\beta} \equiv \frac{\partial^2 U_{ij}}{\partial a_i^\alpha \partial a_j^\beta}, \\ &J_{ij}^{\alpha\beta} \equiv \frac{\partial^2 J_{ij}}{\partial a_i^\alpha \partial a_j^\beta}. \end{aligned}$$

As usual, to close the system of equations, it is necessary to decouple the high-order products of operators. These higher-order operator products, involving the variables of different nature, can be decoupled. Thus, we decouple the atomic and vibrational degrees of freedom involving the second-order vibrational variables:

$$\begin{aligned} u_{ij}^\alpha u_{ij}^\beta c_i^\dagger c_j^\dagger c_j c_i &= \langle u_{ij}^\alpha u_{ij}^\beta \rangle c_i^\dagger c_j^\dagger c_j c_i + u_{ij}^\alpha u_{ij}^\beta \langle c_i^\dagger c_j^\dagger c_j c_i \rangle \\ &\quad - \langle u_{ij}^\alpha u_{ij}^\beta \rangle \langle c_i^\dagger c_j^\dagger c_j c_i \rangle, \\ u_{ij}^\alpha u_{ij}^\beta c_i^\dagger c_j &= \langle u_{ij}^\alpha u_{ij}^\beta \rangle c_i^\dagger c_j + u_{ij}^\alpha u_{ij}^\beta \langle c_i^\dagger c_j \rangle - \langle u_{ij}^\alpha u_{ij}^\beta \rangle \langle c_i^\dagger c_j \rangle, \\ \mathbf{p}_j^2 c_j^\dagger c_j &= \langle \mathbf{p}_j^2 \rangle c_j^\dagger c_j + \mathbf{p}_j^2 \langle c_j^\dagger c_j \rangle - \langle \mathbf{p}_j^2 \rangle \langle c_j^\dagger c_j \rangle. \end{aligned} \tag{26}$$

Such a decoupling is motivated by the different physical nature of the atomic and deviation operators. Keeping in mind the lattice periodicity, the filling factor can be represented as

$$\nu \equiv \frac{N}{N_L} = \frac{1}{N_L}\sum_j \langle c_j^\dagger c_j \rangle = \langle c_j^\dagger c_j \rangle. \tag{27}$$

Employing the above decouplings in the Hamiltonian, we meet the combination of terms, for which it is convenient to introduce the following notations. Thus, we define the effective hopping term

$$\widetilde{J}_{ij} \equiv J_{ij} - \frac{1}{2}\sum_{\alpha\beta} J_{ij}^{\alpha\beta} \langle u_{ij}^\alpha u_{ij}^\beta \rangle \tag{28}$$

and the effective atomic interactions

$$\widetilde{U}_{ij} \equiv U_{ij} - \frac{1}{2}\sum_{\alpha\beta} U_{ij}^{\alpha\beta} \langle u_{ij}^\alpha u_{ij}^\beta \rangle, \tag{29}$$

whose values are renormalized by the presence of atomic vibrations. These atomic vibrations are correlated with each other through the effective interaction matrix

$$\Phi_{ij}^{\alpha\beta} \equiv U_{ij}^{\alpha\beta} \langle c_i^\dagger c_j^\dagger c_j c_i \rangle - 2 J_{ij}^{\alpha\beta} \langle c_i^\dagger c_j \rangle. \tag{30}$$

Atoms produce the effective deformation force

$$F_{ij}^\alpha \equiv -U_{ij}^\alpha c_i^\dagger c_j^\dagger c_j c_i + 2 J_{ij}^\alpha c_i^\dagger c_j, \tag{31}$$

caused by atom-vibration correlations. It is also important to note that for a function $f(\mathbf{a}_{ij})$, depending on the difference $\mathbf{a}_{ij}$, the following properties are valid:

$$\sum_j \frac{\partial f(\mathbf{a}_{ij})}{\partial a_i^\alpha} = \frac{\partial}{\partial a_i^\alpha} \sum_j f(\mathbf{a}_{ij}) = 0,$$
$$\sum_j \frac{\partial^2 f(\mathbf{a}_{ij})}{\partial a_i^\alpha \partial a_j^\beta} = -\frac{\partial}{\partial a_i^\alpha} \sum_j \frac{\partial f(\mathbf{a}_{ij})}{\partial a_{ij}^\beta} = 0. \tag{32}$$

These properties are used in the final presentation of the system Hamiltonian.

Accomplishing the described procedure for Hamiltonian (10), we obtain

$$\hat{H} = E_N + \hat{H}_{\rm at} + \hat{H}_{\rm vib} + \hat{H}_{\rm int}. \tag{33}$$

Here the first term is the nonoperator quantity,

$$E_N = \frac{1}{4} \sum_{i\neq j} \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} \langle u_{ij}^\alpha u_{ij}^\beta \rangle - \nu \sum_j \left\langle \frac{\mathbf{p}_j^2}{2m} \right\rangle. \tag{34}$$

Atoms are described by the renormalized Hamiltonian,

$$\hat{H}_{\rm at} = -\sum_{i\neq j} \widetilde{J}_{ij} c_i^\dagger c_j + \frac{U}{2} \sum_j c_j^\dagger c_j^\dagger c_j c_j + \frac{1}{2} \sum_{i\neq j} \widetilde{U}_{ij} c_i^\dagger c_j c_j c_i + \sum_j \left\langle \frac{\mathbf{p}_j^2}{2m} \right\rangle c_j^\dagger c_j. \tag{35}$$

Collective vibrational degrees of freedom are characterized by the Hamiltonian

$$\hat{H}_{\rm vib} = \nu \sum_j \frac{\mathbf{p}_j^2}{2m} - \frac{1}{4} \sum_{i\neq j} \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} u_{ij}^\alpha u_{ij}^\beta. \tag{36}$$

And the last term $\hat{H}_{\rm int}$ corresponds to local deformations caused by the correlations between atomic and vibrational degrees of freedom,

$$\hat{H}_{\rm int} = -\frac{1}{2} \sum_{i\neq j} \sum_\alpha F_{ij}^\alpha u_{ij}^\alpha. \tag{37}$$

Passing from the relative deviations $\mathbf{u}_{ij}$ to the single-site deviations $\mathbf{u}_j$, and using the above properties, the vibrational Hamiltonian part can be represented as

$$\hat{H}_{\rm vib} = \nu \sum_j \frac{\mathbf{p}_j^2}{2m} + \frac{1}{2} \sum_{i\neq j} \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} u_i^\alpha u_j^\beta. \tag{38}$$

The effective deformation force, (31), enjoys the property

$$F_{ji}^\alpha = -F_{ij}^\alpha \quad (i \neq j). \tag{39}$$

Therefore the deformation term, caused by the correlations between atomic and vibrational degrees of freedom, can be rewritten as

$$\hat{H}_{\rm int} = \sum_{i\neq j} \sum_\alpha F_{ij}^\alpha u_j^\alpha. \tag{40}$$

Thus, all terms of the Hamiltonian $\hat{H}$ are defined.

Let us stress that the vibrational collective excitations appear only when there exist intersite atomic interactions correlating atoms. In the presence of these interactions, atoms move in an effective potential composed of an optical lattice and a self-organized field formed by intersite interactions. The optical lattice does not correlate atoms, prescribing only their individual properties. However, intersite atomic interactions do collectivize the atoms, whose collective vibrations play the role of collective phonon excitations.

IV. QUANTIZATION OF PHONON VARIABLES

Quantized phonon variables are introduced so as to diagonalize the part of the Hamiltonian containing atomic deviations. In our case, the difference from the standard introduction of phonon operators is due to the existence of the linear in the deviation term, (40). Dealing with such linear terms requires us to slightly modify the corresponding canonical transformation [20]. In this case, the phonon operators are introduced by means of the nonuniform transformation

$$\mathbf{u}_j = \vec{\Delta}_j + \frac{1}{\sqrt{2N}} \sum_{ks} \sqrt{\frac{\nu}{m\omega_{ks}}}\, \mathbf{e}_{ks} (b_{ks} + b_{-ks}^\dagger) e^{i\mathbf{k}\cdot\mathbf{a}_j},$$
$$\mathbf{p}_j = -\frac{i}{\sqrt{2N}} \sum_{ks} \sqrt{\frac{m\omega_{ks}}{\nu}}\, \mathbf{e}_{ks} (b_{ks} - b_{-ks}^\dagger) e^{i\mathbf{k}\cdot\mathbf{a}_j}, \tag{41}$$

in which $\mathbf{e}_{ks}$ are the polarization vectors, with s being the polarization index. The phonon frequencies are given by the eigenproblem

$$\frac{\nu}{m} \sum_{j(\neq i)} \sum_\beta \Phi_{ij}^{\alpha\beta} e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} e_{ks}^\beta = \omega_{ks}^2 e_{ks}^\alpha, \tag{42}$$

with the effective interaction matrix, (30). Diagonalizing the phonon part of the Hamiltonian yields

$$\Delta_i^\alpha = \sum_{j(\neq i)} \sum_\beta \gamma_{ij}^{\alpha\beta} F_j^\beta, \tag{43}$$

where we use the notation

$$\gamma_{ij}^{\alpha\beta} \equiv \frac{\nu}{N} \sum_{ks} \frac{e_{ks}^\alpha e_{ks}^\beta}{m\omega_{ks}^2} e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} \tag{44}$$

and where the effective deformation force, acting on an atom, is

$$F_i^\alpha = \sum_{j(\neq i)} F_{ij}^\alpha. \tag{45}$$

The presence of the term $\vec{\Delta}_j$ in the canonical transformation, (41), distinguishes the latter from the standard canonical transformation in the quantization of phonon variables.

It is easy to see that variables (41) satisfy the usual commutation relations,

$$\left[u_i^\alpha,\, p_j^\beta\right] = i\delta_{ij}\delta_{\alpha\beta}.$$

Conditions (22) are valid, since

$$\langle \vec{\Delta}_i \rangle = 0. \tag{46}$$

Then Hamiltonian (33) results in the sum

$$\hat{H} = E_N + \hat{H}_{\rm at} + \hat{H}_{\rm ph} + \hat{H}_{\rm ind}. \tag{47}$$

Here the first term is the same as in Eq. (34). The atomic Hamiltonian is given by Eq. (35). The phonon Hamiltonian is diagonal,

$$\hat{H}_{\rm ph} = \sum_{ks} \omega_{ks} \left(b_{ks}^{\dagger} b_{ks} + \frac{1}{2} \right). \tag{48}$$

And the last term is the Hamiltonian of effective multiatomic interactions, induced by atomic vibrations,

$$\hat{H}_{\rm ind} = \sum_{i \neq j} \sum_{\alpha\beta} F_i^{\alpha} \gamma_{ij}^{\alpha\beta} F_j^{\beta}. \tag{49}$$

Using properties (32), it is straightforward to check that the average force, (45), is 0; that is, $\langle F_j^{\alpha} \rangle = 0$. Hence, the induced term, (49), in the mean-field approximation is 0, $\langle \hat{H}_{\rm ind} \rangle = 0$, since

$$\left\langle F_i^{\alpha} F_j^{\beta} \right\rangle \cong \left\langle F_i^{\alpha} \right\rangle \left\langle F_j^{\beta} \right\rangle = 0.$$

Moreover, the induced term, (49), is much smaller compared to the atomic term, (35). This implies that the induced term (49) does not influence much the properties of atoms.

The properties of phonons depend on their frequency, for which we have the equation

$$\omega_{ks}^2 = \frac{\nu}{m} \sum_{j(\neq i)} \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} e_{ks}^{\alpha} e_{ks}^{\beta} e^{i\mathbf{k}\cdot\mathbf{a}_{ij}}. \tag{50}$$

The deviation correlation function becomes

$$\left\langle u_i^{\alpha} u_j^{\beta} \right\rangle = \delta_{ij} \frac{\nu}{2N} \sum_{ks} \frac{e_{ks}^{\alpha} e_{ks}^{\beta}}{m\omega_{ks}} \coth\left(\frac{\omega_{ks}}{2T} \right). \tag{51}$$

And the average kinetic energy per atom is

$$\left\langle \frac{\mathbf{p}_j^2}{2m} \right\rangle = \frac{1}{4\nu N} \sum_{ks} \omega_{ks} \coth\left(\frac{\omega_{ks}}{2T} \right). \tag{52}$$

An important quantity, characterizing the width of atomic vibrations, is the mean-square deviation r_0 defined by the equation

$$r_0^2 \equiv \sum_{\alpha=1}^{d} \left\langle u_i^{\alpha} u_i^{\alpha} \right\rangle. \tag{53}$$

This quantity should not be confused with l_0, which defines the width of a wave packet at a lattice site: r_0 is the mean deviation of this wave packet oscillating around the lattice site.

In the case of a d-dimensional *cubic* lattice, the frequency is the same for all polarizations, which can be described by the relation

$$\omega_k^2 = \frac{1}{d} \sum_{s=1}^{d} \omega_{ks}^2. \tag{54}$$

The latter results in the equation for the phonon frequency

$$\omega_k^2 = -\frac{\nu}{m} \sum_{j(\neq i)} D_{ij} e^{i\mathbf{k}\cdot\mathbf{a}_{ij}}, \tag{55}$$

with the dynamical matrix

$$D_{ij} \equiv -\frac{1}{d} \sum_{\alpha=1}^{d} \Phi_{ij}^{\alpha\alpha} = \frac{1}{d} \sum_{\alpha=1}^{d} \frac{\partial^2 \Phi_{ij}}{\partial a_i^{\alpha} \partial a_i^{\alpha}}. \tag{56}$$

For a cubic lattice, the mean-square deviation, (53), reads as

$$r_0^2 = \frac{\nu d}{2m\rho} \int_{\mathcal{B}} \frac{1}{\omega_k} \coth\left(\frac{\omega_k}{2T} \right) \frac{d\mathbf{k}}{(2\pi)^d}, \tag{57}$$

with the integration over the Brillouin zone. Taking into account only the nearest-neighbor interactions leads to the effective phonon dispersion

$$\omega_k^2 = \frac{4\nu}{m} D_0 \sum_{\alpha} \sin^2\left(\frac{k_{\alpha} a}{2} \right), \tag{58}$$

where $a_{\alpha} = a$ and D_0 is D_{ij} for the nearest neighbors. In the long-wave limit, Eq. (58) reduces to the acoustic spectrum

$$\omega_k \simeq c_0 k \qquad \left(k^2 \equiv \sum_{\alpha=1}^{d} k_{\alpha}^2 \to 0 \right), \tag{59}$$

with the sound velocity

$$c_0 = \sqrt{\frac{\nu}{m} D_0 a^2}. \tag{60}$$

The value of the mean-square deviation, (57), describes the properties of the localized state and defines the region where it can exist. As is clear, to be treated as localized, the state has to enjoy a mean-square deviation that is much smaller than the mean interatomic distance. This is the essence of the Lindemann criterion of stability that is considered in the next section.

V. POSSIBILITY OF PHONON INSTABILITY

One of the most important characteristics of a localized solid-like state is the mean-square deviation, (53) or (57). A localized state can exist only when this deviation r_0 is much smaller than the distance a between the nearest neighbors. This statement is the well-known *Lindemann criterion of lattice stability* (see, e.g., [18,19,21]). According to this criterion, the majority of solids become unstable and melt when the Lindemann ratio r_0/a surpasses 0.2. This criterion is valid for anharmonic crystals as well [22]. Even for such a strongly anharmonic quantum crystal as ^{3}He the Lindemann ratio is 0.3, which is measured experimentally [23]. In the weakest form, the Lindemann criterion [24] states that, for the stability of a localized solid-like system, it is necessary that

$$\frac{r_0}{a} < 1. \tag{61}$$

The meaning of the Lindemann criterion is evident: if the mean-square deviations of neighboring atoms were comparable to their mean interatomic distance, the system could not be considered localized.

In the long-wave limit, the phonon spectrum is acoustic, as shown in Eq. (59). This tells us that, in calculating the mean-square deviation, (57), the limit of small wave vectors can produce infrared divergence, depending on the system dimensionality and temperature. In order to study when and how this happens, we can employ the standard procedure of limiting integral, (57), from below by introducing the minimal wave vector $k_{\min}$, which is assumed to tend to 0. Equivalently, it is possible to define the minimal wave vector as $k_{\min} = \pi/L$, where $L = aN_L^{1/d}$ is the length of the lattice. As is clear, for a large lattice, with the number of lattice sites $N_L \to \infty$, the minimal wave vector tends to 0.

Considering integral (57) at finite temperatures $T > 0$ for a low dimensionality, $d < 2$, shows that the mean-square deviation diverges as

$$r_0^2 \simeq \frac{T N_L^{2/d-1} d}{2^d \pi^2 (2-d) \nu D_0} \quad (d < 2,\ T > 0),$$

where D_0 is the dynamical matrix, as in Eq. (58), and $N_L \to \infty$. In particular, for one-dimensional space ($d = 1$), the divergence is linear at the number of sites N_L,

$$r_0^2 \simeq \frac{T N_L}{2\pi^2 \nu D_0} \quad (d = 1,\ T > 0). \tag{62}$$

And for two-dimensional space ($d = 2$), the divergence is logarithmic in N_L,

$$r_0^2 \simeq \frac{T \ln N_L}{(2\pi)^2 \nu D_0} \quad (d = 2,\ T > 0). \tag{63}$$

This means that at finite temperatures the localized state is unstable in dimensions $d = 1$ and $d = 2$ for asymptotically large lattices, where $N_L \to \infty$, although the lattice could exist for such N_L that would be large, but finite, at the same time satisfying the Lindemann criterion (61).

Let us note that the dynamical matrix D_0, of course, depends on the parameters of the optical lattice. This is shown below by explicit equations. However, the infrared divergence, considered above, is a feature typical of low-dimensional systems. Recall that, according to the Mermin-Wagner theorem [25–27], continuous symmetry at a finite temperature cannot be broken in spaces of dimensionality lower than 3 ($d \leqslant 2$), irrespective of the strength of their interactions, provided that the latter are of the short-range type. This low-dimensional infrared instability is a purely dimensional effect. However, this low-dimensional effect is not of great danger in a real world that is three-dimensional. Actually, dealing with optical lattices, one always deals with three-dimensional systems, which can be reduced to quasi-one-dimensional or quasi-two-dimensional by integrating out some degrees of freedom.

It is generally accepted that for solid states the Debye approximation gives a quite accurate description [18,19,21–23]. In this approximation, the integration over the Brillouin zone is replaced by the integration over the Debye sphere,

$$\int_{\mathcal{B}} \frac{d\mathbf{k}}{(2\pi)^d} \to \frac{2}{(4\pi)^{d/2}\Gamma(d/2)} \int_0^{k_D} k^{d-1} dk, \tag{64}$$

limited by the Debye radius k_D, which is defined by the normalization condition

$$\int_{\mathcal{B}} \frac{d\mathbf{k}}{(2\pi)^d} = \frac{N_L}{V} = \frac{\rho}{\nu}, \tag{65}$$

where ρ is the average density

$$\rho \equiv \frac{N}{V} = \frac{\nu}{a^d}. \tag{66}$$

This gives the Debye radius

$$k_D = \frac{\sqrt{4\pi}}{a} \left[\frac{d}{2}\, \Gamma\left(\frac{d}{2}\right) \right]^{1/d}. \tag{67}$$

The spectrum is taken to be isotropic, with the frequency

$$\omega_k = c_0 k \quad (0 \leqslant k \leqslant k_D), \tag{68}$$

whose upper limit defines the Debye temperature

$$T_D \equiv c_0 k_D. \tag{69}$$

With the notation for the Debye radius, (67), the replacement, (64), takes the form

$$\int_{\mathcal{B}} \frac{d\mathbf{k}}{(2\pi)^d} \to \frac{d}{(k_D a)^d} \int_0^{k_D} k^{d-1} dk. \tag{70}$$

Below, we study in more detail the Lindemann criterion, employing the Debye approximation.

At zero temperature, the mean-square deviation becomes

$$r_0^2 = \frac{d^2}{2(d-1) m T_D} \quad (T = 0). \tag{71}$$

The Lindemann criterion of stability, (61), yields

$$T_D > \frac{d^2}{2(d-1) m a^2} \quad (T = 0). \tag{72}$$

The meaning of the latter inequality is very transparent: a localized state can be formed only when the effective potential energy is higher than the kinetic energy of atoms. As Eq. (72) demonstrates, no localized state can exist at zero temperature for $d = 1$.

At high temperatures, the mean-square deviation is given by the expression

$$r_0^2 \simeq \frac{T d^2}{(d-2) m T_D^2} \quad (T \gg T_D). \tag{73}$$

Then the Lindemann stability criterion gives

$$T_D > \sqrt{\frac{T d^2}{(d-2) m a^2}} \quad (T \gg T_D). \tag{74}$$

This tells us that, at such temperatures, there can be no localized state for $d = 2$. At these temperatures, only a three-dimensional localized state can exist, provided that

$$T_D > \sqrt{\frac{9T}{ma^2}} \quad (T > T_D,\ d = 3). \tag{75}$$

To simplify the consideration, for a well-localized insulating state, one can use the averages $\langle c_i^\dagger c_j \rangle = \delta_{ij} \nu$ and

$$\langle c_i^\dagger c_j^\dagger c_j c_i \rangle = \langle c_i^\dagger c_i \rangle \langle c_j^\dagger c_j \rangle = \nu^2 \quad (i \neq j). \tag{76}$$

As a result, the interaction matrix, (30), reduces to

$$\Phi_{ij}^{\alpha\beta} = \nu^2 U_{ij}^{\alpha\beta}. \tag{77}$$

An interesting question is how atomic vibrations influence a localized state due to local interactions. For such a case, considering a cubic lattice, taking account of only the nearest neighbors, and involving the formulas from Appendix A, we get

$$U_{ij} = U \exp\left(-\frac{a^2 d}{2l_0^2}\right), \tag{78}$$

where the equality $a_{ij}^2 = a^2 d$ is used and $U = U_{\rm loc}$ is defined in Appendix A. The dynamical matrix, (56), becomes

$$D_0 = \left(\frac{\nu a}{l_0^2}\right)^2 U \exp\left(-\frac{a^2 d}{2l_0^2}\right). \tag{79}$$

The sound velocity, (60), reads as

$$c_0 = \frac{\nu a^2}{l_0^2}\sqrt{\frac{\nu}{m}U}\exp\left(-\frac{a^2 d}{4l_0^2}\right), \tag{80}$$

which can also be represented in the form

$$c_0 = \frac{4\nu J a^2}{(\pi^2-4)V_0 l_0^2 d}\sqrt{\frac{\nu}{m}U}, \tag{81}$$

through the parameters of the optical lattice.

For a cubic lattice at zero temperature, the Lindemann criterion of stability, (61), can be written as

$$\frac{16(2\pi)^{1/4}\nu^{3/2}J}{(\pi^2-4)V_0 d}\left[\frac{d}{2}\Gamma\left(\frac{d}{2}\right)\right]^{1/d}\left(\frac{a}{l_0}\right)^3\sqrt{\frac{a_{\rm eff}}{l_\perp^{3-d}l_0^{d-2}}} > \frac{d^2}{d-1}. \tag{82}$$

Consequently, the system stability essentially depends on the lattice parameters, space dimensionality, and atomic interactions.

At zero temperature, only two- and three-dimensional localized states can arise. Considering the two-dimensional case ($d = 2$), we have

$$\Phi_2 = \frac{\Phi_{\rm eff}}{\sqrt{2\pi}l_\perp}, \quad k_D = \frac{\sqrt{4\pi}}{a}, \quad U = \frac{\Phi_{\rm eff}}{(2\pi)^{3/2}l_\perp l_0^2} \quad (d=2). \tag{83}$$

The Debye temperature, (69), becomes

$$T_D = 2(2\pi)^{1/4}\frac{\nu a}{m l_0^3}\sqrt{\frac{\nu a_{\rm eff}}{l_\perp}}\exp\left(-\frac{a^2}{2l_0^2}\right). \tag{84}$$

The Lindemann criterion, (72), is equivalent to the inequality

$$ma^2 T_D > 2,$$

which gives

$$\nu^{3/2}\left(\frac{a}{l_0}\right)^3\sqrt{\frac{a_{\rm eff}}{l_\perp}}\exp\left(-\frac{a^2}{2l_0^2}\right) > 0.632. \tag{85}$$

Comparing the ratio $U_{\rm loc}/J$, given in Appendix A, with criterion (85), we see that the atomic state can be insulating when no phonon degrees of freedom are taken into account and U is much larger than J. But as soon as phonon excitations are included, the stability condition, (85), for the same parameters may not be valid, which means that atoms delocalize.

For the three-dimensional case ($d = 3$), we get

$$\Phi_3 = \Phi_0, \quad k_D = \frac{(6\pi^2)^{1/3}}{a}, \quad U = \frac{\Phi_0}{(2\pi)^{3/2}l_0^3} \quad (d=3). \tag{86}$$

The Debye temperature, (69), becomes

$$T_D = 3.482\frac{\nu a}{m l_0^3}\sqrt{\frac{\nu a_s}{l_0}}\exp\left(-\frac{3a^2}{4l_0^2}\right). \tag{87}$$

At zero temperature, the Lindemann criterion, (72), takes the form

$$ma^2 T_D > \frac{9}{4},$$

which yields

$$\nu^{3/2}\left(\frac{a}{l_0}\right)^3\sqrt{\frac{a_s}{l_0}}\exp\left(-\frac{3a^2}{4l_0^2}\right) > 0.648. \tag{88}$$

Again, the system can be insulating without phonons, but becomes delocalized in the presence of the latter.

Using the formulas in Appendix A, localization conditions (85) and (88) can be represented in another form by taking into account the expressions for the hopping rate,

$$J = 2.935 V_0 \exp\left(-\frac{a^2}{2l_0^2}\right) \quad (d=2),$$

$$J = 4.402 V_0 \exp\left(-\frac{3a^2}{4l_0^2}\right) \quad (d=3).$$

Then Eq. (85) yields

$$\frac{a_{\rm eff}}{l_\perp} > \frac{3.441}{\nu^3}\left(\frac{V_0}{J}\right)^2\left(\frac{l_0}{a}\right)^6 \quad (d=2), \tag{89}$$

while criterion (88) gives

$$\frac{a_s}{l_0} > \frac{8.137}{\nu^3}\left(\frac{V_0}{J}\right)^2\left(\frac{l_0}{a}\right)^6 \quad (d=3). \tag{90}$$

This shows that the Lindemann criterion of stability requires that atomic interactions, and hence the scattering length, be sufficiently large. If these conditions are not valid, the insulating state can be destroyed by phonon vibrations.

In order to better understand the physics of the phonon instability, we need to analyze how the occurrence of atomic vibrations influences the values of the hopping parameter and interaction matrix.

VI. RENORMALIZATION OF ATOMIC PARAMETERS

Phonon excitations renormalize atomic parameters according to Eqs. (28) and (29). The renormalized quantities are shifted, because of the phonon existence, resulting in

$$\widetilde{J}_{ij} = J_{ij} + \Delta J_{ij}, \quad \widetilde{U}_{ij} = U_{ij} + \Delta U_{ij}, \tag{91}$$

where, taking into account that

$$\langle u_{ij}^{\alpha} u_{ij}^{\beta}\rangle = 2(1-\delta_{ij})\langle u_i^{\alpha} u_j^{\beta}\rangle,$$

we have

$$\Delta J_{ij} = -\sum_{\alpha\beta} J_{ij}^{\alpha\beta}\langle u_j^{\alpha} u_j^{\beta}\rangle, \quad \Delta U_{ij} = -\sum_{\alpha\beta} U_{ij}^{\alpha\beta}\langle u_j^{\alpha} u_j^{\beta}\rangle. \quad (92)$$

In the Debye approximation, we find

$$\langle u_j^{\alpha} u_j^{\beta}\rangle = \delta_{\alpha\beta}\frac{r_0^2}{d}, \quad (93)$$

which gives

$$\Delta J_{ij} = -\frac{r_0^2}{d}\sum_{\alpha} J_{ij}^{\alpha\alpha}, \quad \Delta U_{ij} = -\frac{r_0^2}{d}\sum_{\alpha} U_{ij}^{\alpha\alpha}. \quad (94)$$

In the tight-binding approximation, where $l_0 \ll a$, the hopping parameter shift is

$$\Delta J_{ij} = \frac{a^2 r_0^2}{4 l_0^4} J_{ij}, \quad (95)$$

which shows that the hopping parameter increases due to collective phonon excitations. At zero temperature, the relative shift is

$$\frac{\Delta J_{ij}}{J_{ij}} = \frac{a^2 d^2}{8(d-1) m l_0^4 T_D}. \quad (96)$$

For a two-dimensional lattice ($d = 2$), this gives

$$\frac{\Delta J_{ij}}{J_{ij}} = 0.079\frac{a}{\nu l_0}\sqrt{\frac{l_\perp}{\nu a_{\rm eff}}}\exp\left(\frac{a^2}{2l_0^2}\right) = 0.074\frac{a V_0}{\nu^{3/2} l_0 J}\sqrt{\frac{l_\perp}{a_{\rm eff}}}, \quad (97)$$

and for a three-dimensional lattice ($d = 3$), the relative shift is

$$\frac{\Delta J_{ij}}{J_{ij}} = 0.054\frac{a}{\nu l_0}\sqrt{\frac{l_0}{\nu a_s}}\exp\left(\frac{3a^2}{4l_0^2}\right) = 0.237\frac{a V_0}{\nu^{3/2} l_0 J}\sqrt{\frac{l_0}{a_s}}. \quad (98)$$

The increase in the hopping parameter can be rather noticeable. Thus, for $r_0/l_0 \sim 0.3$ and $l_0/a \sim 0.1$, shift (95) is of the order of J_{ij}.

The shift of the interaction matrix with the local interaction potential reads as

$$\Delta U_{ij} = \frac{a^2 r_0^2}{l_0^4} U_{ij}, \quad (99)$$

which means that the interaction matrix increases. At zero temperature, this yields

$$\frac{\Delta U_{ij}}{U_{ij}} = \frac{a^2 d^2}{2(d-1) m l_0^4 T_D}. \quad (100)$$

The increase in the effective interaction matrix U_{ij}, caused by collective phonon excitations, can be sufficiently large, even in the case of the local atomic interactions. For instance, if $r_0/l_0 \sim 0.3$ and $l_0/a \sim 0.1$, then shift (99) is of the order of U_{ij}. Thus, the phonon vibrations can essentially renormalize the atomic Hamiltonian parameters. A simple example of temperature dependence is given in Appendix B.

In this way, collective phonon excitations lead to an increase in the hopping parameter and in the interaction matrix corresponding to the interactions of atoms at different lattice sites. However, note that the on-site atomic interaction parameter U in Hamiltonian (35) remains unchanged.

VII. PHYSICS OF PHONON INSTABILITY

Now it is straightforward to understand why collective phonon excitations can lead to the instability of an insulating state. To this end, keeping in mind low temperatures, let us compare the energy of the system described by the Hamiltonian without phonon degrees of freedom with the energy of the system including phonon excitations. These energies are given by the average values of the related Hamiltonians. The energy of the system with phonons is defined as the average $\tilde{E} \equiv \langle \hat{H}\rangle$ of Hamiltonian (33), while the energy E of the system without phonons can be defined as the average of Hamiltonian (10). So, we need to consider the difference $\Delta \equiv \tilde{E} - E$.

As explained above, analyzing the interaction Hamiltonian, (40), we find that its average value is small, $\langle \hat{H}_{\rm int}\rangle \approx 0$. Appendix A shows that the intersite term U_{ij}, with $i \neq j$, is much smaller than the on-site term U. Thus, we obtain the energy difference

$$\Delta E \approx -\sum_{i\neq j} \Delta J_{ij}\langle c_i^{\dagger} c_j\rangle.$$

In the previous section, it is shown that the hopping parameter shift is positive. Thus, the existence of phonons increases the hopping parameter and, consequently, decreases the system energy. Since the system with phonons prefers a lower energy, it is more stable than the system without these excitations.

A localized state is metastable, since in order to destroy it, atoms have to penetrate through the barrier V_0 created by the optical lattice. Such a penetration requires some time, which characterizes the lifetime of the metastable state. This lifetime can be estimated [28–32] as

$$t_{\rm met} = \tau_0 \exp\left(\frac{V_B}{\varepsilon_N}\right),$$

where V_B is the barrier height, ε_N is the characteristic energy of noise, which is defined by the characteristic kinetic energy, and τ_0 is the period of atomic oscillations at the bottom of the well. For classical systems the characteristic noise energy ε_N coincides with the temperature T, which results in the Arrhenius formula. For quantum systems, the characteristic kinetic energy is defined by the energy, which, in our case, is the recoil energy E_R. And the barrier height for an optical lattice is V_0. With the oscillation period $\tau = 2\pi/\omega_0$, we have the lifetime

$$t_{\rm met} = \frac{2\pi}{\omega_0}\exp\left(\frac{V_0}{E_R}\right).$$

As an illustration of the above consideration, let us study some experiments where the insulating state in an optical lattice has been observed. For example, let us consider the experiment by Greiner *et al.* [33], where a three-dimensional cubic lattice was created and loaded with ^{87}Rb atoms, with the filling number close to 1. Varying the optical-lattice

parameters, both localized insulating and delocalized superfluid states were realized. The lattice was formed by laser beams of wavelength $\lambda = 0.852 \times 10^{-4}$ cm, which makes the lattice parameter $a = \lambda/2 = 0.426 \times 10^{-4}$ cm. With mass $m = 1.443 \times 10^{-22}$ g, the recoil energy is $E_R = 2.093 \times 10^{-23}$ erg. At lattice depth $V_0 = 13E_R = 2.721 \times 10^{-22}$ erg, atoms are localized in a Mott state. Under these parameters, the effective frequency $\omega_0 = 1.509 \times 10^{-22}$ erg, which gives the wave packet width $l_0 = 0.715 \times 10^{-5}$ cm. Since $l_0/a = 0.168$, the tight-binding approximation is applicable. With the scattering length $a_s = 0.545 \times 10^{-6}$ cm, we have the ratio $a_s/l_0 = 0.076$.

At the same time, for $V_0 = 13E_R$ numerical calculations [33] give $U = 0.35E_R$ and $J = U/36 = 0.97 \times 10^{-2}E_R$. Then the Lindemann criterion, (90), requires that a_s/l_0 be larger than 330. According to this criterion, the localized insulating state is unstable if the phonon degrees of freedom are taken into account. Therefore, the experimentally observed localized states of atoms interacting through local δ-function forces are not absolutely stable equilibrium states but, rather, are metastable states.

The oscillation time of an atom in a well is $\tau = 2\pi/\omega_0 = 0.44 \times 10^{-3}$ s. Therefore, the lifetime of a metastable insulating state under $V_0 = 13E_R$ is $t_{\rm met} \approx 200$ s. This is quite a long time, allowing for its easy observation. Moreover, this time is longer than the typical lifetime of atoms in a trap, which is of the order of seconds or tens of seconds [34,35]. Therefore, it is very feasible to create long-lived metastable insulating states of trapped atoms in optical lattices.

VIII. ATOMS WITH DIPOLE INTERACTIONS

In the case of nonlocal long-range atomic interactions $\Phi_{\rm non}(\mathbf{r})$, such as dipolar interactions, atoms in an optical lattice, where $l_0 \ll a$, can be described [5–8] by the extended Hubbard model with the effective interactions

$$U_{ij} = \frac{C_D}{a_{ij}^3} \quad (i \neq j), \tag{101}$$

in which $C_D \propto \mu_0^2$, with μ_0 being the magnetic (or electric) atomic dipole. Since dipole interactions are of the hard-core type, each lattice site can host only a single atom; that is, the filling factor is 1, $\nu = 1$. For interactions of form (101), one has

$$U_{ij}^{\alpha} = -3C_d\,\frac{a_{ij}^{\alpha}}{a_{ij}^5}, \quad U_{ij}^{\alpha\beta} = \frac{3C_d}{a_{ij}^5}\left(\delta_{\alpha\beta} - \frac{5a_{ij}^{\alpha}a_{ij}^{\beta}}{a_{ij}^2}\right).$$

The shift of the effective interactions due to phonon excitations, according to Eq. (94), reads as

$$\Delta U_{ij} = \frac{3(5-d)}{d} r_0^2 \frac{C_D}{a_{ij}^5}. \tag{102}$$

Taking into account only nearest neighbors yields

$$\Delta U_{ij} = \frac{3(5-d)}{d^2}\left(\frac{r_0}{a}\right)^2 U_{ij}. \tag{103}$$

Again, we see that the presence of phonons increases effective interactions. This increase is not large, since, for $r_0 \ll a$, Eq. (103) shows that the shift is much smaller than U_{ij}.

For a well-localized insulating state, the interaction matrix, (30), leads to

$$\Phi_{ij}^{\alpha\beta} = 3\frac{U_{ij}}{a_{ij}^2}\left(\delta_{\alpha\beta} - \frac{5a_{ij}^{\alpha}a_{ij}^{\beta}}{a_{ij}^2}\right), \tag{104}$$

which defines the dynamical matrix, (56), as

$$D_{ij} = \frac{3(5-d)}{d}\frac{U_{ij}}{a_{ij}^2}. \tag{105}$$

Taking into account only nearest neighbors gives

$$D_0 = \frac{3(5-d)}{d^{7/2}}\,\frac{C_D}{a^5}. \tag{106}$$

The sound velocity, (60), becomes

$$c_0 = \left[\frac{3(5-d)C_D}{ma^3 d^{7/2}}\right]^{1/2},$$

which, for the Debye temperature, (69), yields

$$T_D = \frac{2\sqrt{3\pi(5-d)}}{d^{7/2}}\left[\frac{d}{2}\Gamma\left(\frac{d}{2}\right)\right]^{1/d}\sqrt{\frac{C_D}{ma^5}}. \tag{107}$$

In particular, for two and three dimensions, we find

$$\begin{aligned} T_D &= 3.162\sqrt{\frac{C_D}{ma^5}} \quad (d=2), \\ T_D &= 1.396\sqrt{\frac{C_D}{ma^5}} \quad (d=3). \end{aligned} \tag{108}$$

It is convenient to introduce the *dipole length*

$$a_D \equiv \frac{mC_D}{\hbar^2}, \tag{109}$$

which is sometimes also called the effective dipole scattering length. Then the Lindemann criterion, (61), for the stability of a localized state can be written, depending on the dimensionality, as

$$\frac{a_D}{a} > 0.4 \quad (d=2), \quad \frac{a_D}{a} > 2.6 \quad (d=3). \tag{110}$$

This tells us that the effective atomic interaction, i.e., the dipole length, has to be sufficiently strong for the stability of the localized state.

In order to estimate the characteristic interaction parameters, let us consider the systems of cold trapped atoms of ^{52}Cr [36], ^{168}Er [37], and ^{164}Dy [38]. We keep in mind that the typical nearest-neighbor distance in an optical lattice is $a \sim 10^{-5}$ cm.

The dipole magnetic moment of ^{52}Cr is $\mu_0 = 6\mu_B$, which gives $\mu_0 = 5.564 \times 10^{-20}$ erg/G. The atomic mass is $m = 0.863 \times 10^{-22}$ g. The scattering length is $a_s = 103a_B$. The sound velocity is $c_0 \sim 0.2$ cm/s. The Debye frequency is $\omega_D \sim 0.6 \times 10^5$ 1/s. The Debye temperature is $T_D \sim 0.7 \times 10^{-22}$ erg or $T_D \sim 0.5 \times 10^{-6}$ K. Taking $C_D \sim \mu_0^2$, we get $a_D = 2.4 \times 10^{-7}$ cm. This is much shorter than the typical lattice distance a. That is, the stability criterion, (110), cannot be satisfied.

For ^{168}Er, the dipole moment is $\mu_0 = 7\mu_B$, which yields $\mu_0 = 6.492 \times 10^{-20}$ erg/G. The mass is $m = 2.777 \times 10^{-22}$ g. Then the dipole length is $a_D = 1.052 \times 10^{-6}$ cm.

This is also shorter than the typical intersite distance a. Hence the stability criterion, (110), is again not valid.

In the case of ^{164}Dy, the dipole moment is $\mu_0 = 10\mu_B$, which results in $\mu_0 = 9.274 \times 10^{-20}$ erg/G. The mass is $m = 2.698 \times 10^{-22}$ g. This gives the dipole length $a_D = 2.087 \times 10^{-6}$ cm, which, again, does not satisfy the stability criterion, (110).

Thus, phonon excitations do not allow for the formation of localized states for the above atoms with pure dipolar forces. But there exist polar molecules for which magnetic (or electric) moments can reach $100\mu_B$ [7]. Such polar molecules, with dipolar lengths several orders larger than those of the above atoms, can satisfy the stability criterion and, hence, can form localized states that are stable against phonon collective excitations. And even when absolutely stable states are not allowed, there can exist very long-lived metastable states.

IX. CONCLUSION

We have studied the influence of phonon collective excitations on the possibility of cold atoms' forming localized states in optical lattices. The phonon excitations that appear are self-organized atomic fluctuations, caused by intersite atomic interactions collectivizing the atoms.

It turns out that such phonon excitations are very important even for atoms with local δ-function interactions. Phonon oscillations can destroy the insulating state that would exist without them. The physical mechanism by which phonons can destabilize an insulating state is the fact that phonons decrease the system energy by increasing the hopping parameter.

The localized state can be stabilized by strong atomic interactions. These conclusions are valid for both local and long-range dipolar interactions. Taking into account collective phonon excitations is necessary when studying whether cold atoms in optical lattices can form localized insulating states in equilibrium. Even though at absolute equilibrium a localized state cannot exist, being unstable with respect to phonon excitations, this does not prohibit the existence of metastable localized states in optical lattices which live so long that they can be easily observed and studied.

The reason why the conditions for the existence of localized states for a pure Hubbard model without phonons and one with phonon excitations are different is easy to understand. In a pure Hubbard model, the state is localized when the width l_0 of the wave packet at a lattice site is narrow, such that it is much smaller than the intersite distance a, or when $k_0 l_0 \ll 1$. The latter, since $k_0 l_0 = (E_R/V_0)^{1/4}$, implies that $V_0 \gg E_R$. Exactly this condition is observed in experiments studying the insulating Mott state in optical lattices [1–4,33].

However, the wave packet can be narrow but strongly oscillating around a lattice site. Such oscillations are characterized by the mean-square deviation r_0. Then the localized state can exist if these oscillating wave packets do not intersect with each other, which is the meaning of the Lindemann criterion of stability, requiring that r_0/a be at least smaller than 1. The latter imposes the condition that atomic interactions be sufficiently strong, satisfying inequality (89) or (90), depending on the space dimensionality. The condition $l_0 \ll a$ does not directly involve the parameters of intersite atomic interactions, while the Lindemann criterion of instability strongly depends on the parameters of such interactions. This is why these criteria are principally different and do not need to coincide.

ACKNOWLEDGMENTS

One of the authors (V.I.Y.) acknowledges financial support from the Augsburg University and from the Russian Foundation for Basic Research (Grant No. 14-02-00723).

APPENDIX A: HOPPING TERM AND INTERSITE INTERACTION

In deriving the extended Hubbard Hamiltonian, one employs the basis of Wannier functions. It is known that this basis is convenient because Wannier functions can be made well localized [39–41], such that the tight-binding approximation becomes applicable, when the Wannier functions are close to harmonic wave packets,

$$w(\mathbf{r}) = \prod_{\alpha=1}^{d} w_\alpha(\mathbf{r}), \quad w_\alpha(\mathbf{r}) = \left(\frac{m\omega_\alpha}{\pi}\right)^{1/4} \exp\left(-\frac{m}{2}\omega_\alpha r_\alpha^2\right).$$

The wave packets are well localized in the sense that

$$\frac{l_\alpha}{a_\alpha} \ll 1 \quad \left(l_\alpha \equiv \frac{1}{\sqrt{m\omega_\alpha}}\right)$$

or, in other words, that

$$k_0^\alpha l_\alpha \ll 1 \quad \left(k_0^\alpha a_\alpha = \pi\right).$$

The value l_α plays the role of the localization length, or width, for the wave packet. The corresponding oscillator frequency ω_α can be found by minimizing the energy of the whole atomic system [4], which takes into account atomic interactions. When the packet width is mainly defined by the optical potential, then

$$\omega_\alpha = \sqrt{\frac{2}{m} V_\alpha k_0^\alpha} \quad \left(k_0^\alpha \equiv \frac{\pi}{a_\alpha}\right).$$

In this approximation, the hopping term, (6), is

$$J_{ij} = \sum_{\alpha=1}^{d} \left[\frac{\omega_\alpha}{8}\left(\frac{a_{ij}^\alpha}{l_\alpha}\right)^2 - V_\alpha\right] \exp\left\{-\frac{1}{4}\sum_{\alpha=1}^{d}\left(\frac{a_{ij}^\alpha}{l_\alpha}\right)^2\right\}$$

and the matrix element, (14), becomes

$$U_{ij}^{\rm loc} = \frac{\Phi_d}{(2\pi)^{d/2}}\left(\prod_{\alpha=1}^{d}\frac{1}{l_\alpha}\right) \exp\left\{-\frac{1}{2}\sum_{\alpha=1}^{d}\left(\frac{a_{ij}^\alpha}{l_\alpha}\right)^2\right\},$$

with the notation

$$\mathbf{a}_{ij} \equiv \mathbf{a}_i - \mathbf{a}_j = \left\{a_{ij}^\alpha\right\}, \quad a_{ij}^2 \equiv |\mathbf{a}_{ij}|^2 = \sum_{\alpha=1}^{d}\left(a_{ij}^\alpha\right)^2.$$

For a cubic lattice, with $V_\alpha = V_0$, $\omega_\alpha = \omega_0$, and $l_\alpha = l_0$, the hopping term simplifies to

$$J_{ij} = \left(\frac{\omega_0 a_{ij}^2}{8 l_0^2} - V_0 d\right) \exp\left(-\frac{a_{ij}^2}{4 l_0^2}\right),$$

while the above intersite interaction becomes

$$U_{ij}^{\rm loc} = U_{\rm loc} \exp\left(- \frac{a_{ij}^2}{2l_0^2} \right),$$

with the on-site interaction, due to the local potential, being

$$U_{\rm loc} = \frac{\Phi_d}{(2\pi)^{d/2} l_0^d}.$$

For a cubic lattice, with the frequency ω_0 defined by the optical potential, we have

$$\omega_0 = 2\sqrt{V_0 E_R} = \frac{\pi}{a}\sqrt{\frac{2}{m} V_0}$$

and

$$l_0 \equiv \frac{1}{\sqrt{m\omega_0}} = \frac{1}{(4m^2 V_0 E_R)^{1/4}},$$

with $E_R = \pi^2/2ma^2$. In the case of the nearest neighbors, using the relations

$$\frac{\omega_0 a_{ij}^2}{8l_0^2} = \frac{\pi^2}{4} V_0 d, \quad l_0^2 = \frac{a}{\pi\sqrt{2mV_0}}, \quad \frac{a^2}{l_0^2} = \pi^2 \sqrt{\frac{V_0}{E_R}},$$

we find the hopping term

$$J = V_0 d \left(\frac{\pi^2}{4} - 1 \right) \exp\left(-\frac{a^2 d}{4l_0^2} \right)$$

and the on-site interaction, caused by the local potential,

$$U_{\rm loc} = \frac{\Phi_d}{\pi^{d/2}} (m^2 V_0 E_R)^{d/4} = \frac{2\omega_0 a_{\rm eff}}{\sqrt{2\pi} l_\perp^{3-d} l_0^{d-2}}.$$

The ratio of the on-site interaction to the hopping term reads as

$$\frac{U_{\rm loc}}{J} = \frac{4\Phi_d \exp\left(a^2 d/4l_0^2\right)}{(\pi^2 - 4)(2\pi)^{d/2} l_0^d \; V_0 d},$$

or it may be presented as

$$\frac{U_{\rm loc}}{J} = \frac{4\Phi_d}{(\pi^2 - 4)d} \left(\frac{m}{2a^2 V_0^3} \right)^{d/4} \exp\left(\frac{\pi d}{4} \sqrt{2mV_0} \right).$$

This shows that, for a sufficiently deep lattice and large scattering length, the value of $U_{\rm loc}$ can be made much larger than J, so that the system would be in a well-localized insulating state.

APPENDIX B: MEAN-FIELD ILLUSTRATION OF PHONON INSTABILITY

The conventional approach to determining the properties of both phonons and atoms is based on a self-consistent evaluation of the self-energy (Migdal approximation) [42]. The latter provides an effective (or renormalized) energy and its imaginary part, an effective scattering rate. Such a static approximation might be insufficient, since it does not take into account thermal fluctuations. It is possible to treat quantum and thermal fluctuations separately. To this end, we can replace the phonon operators b_{ks} and $b_{ks}^\dagger$ in (41) with their quantum averages: $b_{ks} \approx \langle b_{ks} \rangle \equiv v_{ks}$ and $b_{ks}^\dagger \approx \langle b_{ks}^\dagger \rangle \equiv v_{ks}^*$. In this approximation, we can keep thermal fluctuations but ignore quantum fluctuations of the phonons. The atoms, on the other hand, are studied in full quantum dynamics. This reduces the grand-canonical ensemble at inverse temperature $\beta \equiv 1/k_B T$, defined by the generating function $\mathrm{Tr} e^{-\beta H}$, to a functional integral with respect to thermal fluctuations of the lattice distortions $\mathbf{u}_j$ and a trace with respect to the quantum states of the atoms [43].

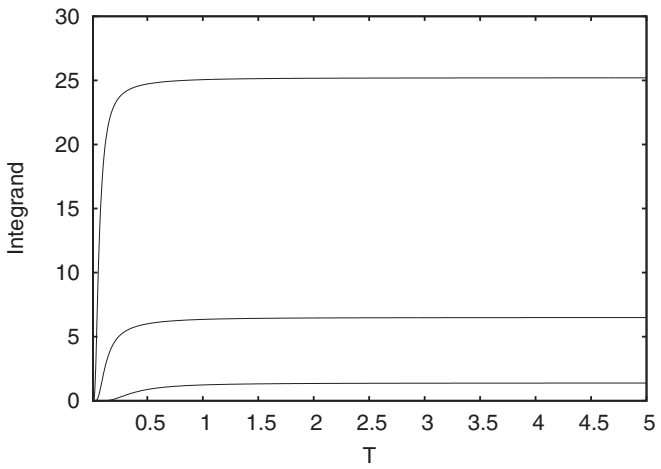

FIG. 1. Integrand of the last equation in Appendix B as a function of temperature T (in units of the hopping energy), describing the increase in phonon fluctuations with rising temperature, for $\sqrt{h_1^2 + h_2^2} = 0.01$, 0.8, and 1 (from bottom to top), $d = 3$, and $\mu = 1.2$.

In order to illustrate how phonon instability can develop, we consider a simplified model to show how phonon fluctuations rise with temperature. For this purpose we choose as the effective quasiatom Hamiltonian h a hopping term and a term that describes the displacement of atoms at nearest-neighbor sites. Assuming a bipartite lattice, the atomic Hamiltonian $\hat{H}_{\rm at}$ of Eq. (35) can be reduced to the effective form

$$h = \begin{pmatrix} \mu & h_1 - ih_2 \\ h_1 + ih_2 & \mu \end{pmatrix},$$
$$h_1 = \left(\hat{H}_{\rm at} + \hat{H}_{\rm at}^T\right)/2, \quad h_2 = i\left(\hat{H}_{\rm at} - \hat{H}_{\rm at}^T\right)/2,$$

where μ is the effective chemical potential of atoms. Within the mean-field approximation, this leads to a spatially uniform displacement field u entering the action

$$S = \beta \hat{H}_{\rm vib} + \int \ln\left[1 + e^{-2\beta\mu} - 2e^{-\beta\mu} \cosh\left(\beta\sqrt{h_1^2 + h_2^2}\right)\right] \times \frac{d\mathbf{k}}{(2\pi)^d},$$

with the phonon Hamiltonian of Eq. (38). Calculation of the phonon free energy $-\beta \ln Z$ requires integration over the atomic displacement field u, which can be performed in the saddle-point approximation fixing the displacement field by

the saddle-point equation

$$0 = \frac{\partial S}{\partial u^\alpha} = \beta \frac{\partial \hat{H}_{\rm vib}}{\partial u^\alpha} - \int \frac{\sinh\left(\beta\sqrt{h_1^2+h_2^2}\right)}{\cosh(\beta\mu) - \cosh\left(\beta\sqrt{h_1^2+h_2^2}\right)} \times \frac{h_1\partial h_1/\partial u^\alpha + h_2\partial h_2/\partial u^\alpha}{\sqrt{h_1^2+h_2^2}} \frac{d\mathbf{k}}{(2\pi)^d}.$$

Phonon fluctuations around the saddle point are described by the fluctuation matrix

$$\frac{\partial^2 S}{\partial u^\alpha \partial u^\beta} = \beta \frac{\partial^2 \hat{H}_{\rm vib}}{\partial u^\alpha \partial u^\beta} - \beta^2 \int \frac{\cosh\left(\beta\sqrt{h_1^2+h_2^2}\right)\cosh(\beta\mu) - 1}{\left[\cosh(\beta\mu) - \cosh\left(\beta\sqrt{h_1^2+h_2^2}\right)\right]^2} \times \frac{(h_1\partial h_1/\partial u^\alpha + h_2\partial h_2/\partial u^\alpha)(h_1\partial h_1/\partial u^\beta + h_2\partial h_2/\partial u^\beta)}{h_1^2+h_2^2} \times \frac{d\mathbf{k}}{(2\pi)^d}.$$

The effect of the phonon fluctuations increases with decreasing eigenvalues of the fluctuation matrix. The negative sign in front of the positive integral reflects the fact that the phonon fluctuations increase with increasing temperature and can eventually lead to an instability of the atomic system. Thus, the fluctuation matrix is related to the Lindemann criterion in Sec. V. This behavior is depicted by the temperature dependence of the integrand in Fig. 1. Eigenvalues can even become negative, which indicates a phase transition. The latter could be either a structural phase transition of the lattice [44,45] or a melting transition [24].

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