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Phonon instability of insulating states in optical lattices

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Abstract. The influence of collective phonon excitations, due to intersite atomic interactions, on the stability of optical lattices is analyzed. These phonon excitations are shown to essentially reduce the ability of atoms to be localized. The states that seem to be insulating in the absence of the phonon excitations can become delocalized when the latter are present. The delocalization effect exists for both long-range as well as local atomic interactions.

1. Introduction

Physics of cold atoms in optical lattices is an intensive field of research, as can be inferred from the review articles [1–5]. Depending on the depth of the wells at the lattice sites, temperature, and interaction strength, atoms can be in an insulating localized state or in delocalized itinerant state. Here we consider insulating states.

In an insulating state, an atom, localized at a lattice-site well, being in the ground state, is described by a well localized atomic wave function, as in Fig. 1a. This function can exhibit two types of variations. First, the wave function of the ground state can be transformed into an excited state, e.g., as is pictured in Fig. 1b, which corresponds to a single-particle excitation. Second, because of interactions with other atoms, the wave packet can oscillate around the lattice site, as is shown in Fig. 1c, which manifests collective phonon excitations.

Thus, in physical reality, there always exist two types of atomic motion, the transfer between different energy levels, accompanied by an essential wave function deformation, and small oscillations around a lattice site, preserving the wave-function shape.

If one postulates that the system is described by a Hubbard Hamiltonian, this implies that small oscillations are disregarded and only transitions between energy bands are taken into account. The Hubbard model is formulated in terms of single-particle states and does not contain collective atomic fluctuations. Clearly, there are no phonon excitations in the standard Hubbard model. However, one should not confuse a model and the physical reality. It is well known that in any real physical system, whether it is gas, liquid, or solid, there always exist sound waves caused by particle interactions. And this does not depend on the presence or absence of any external fields. In nature, any realistic physical system of interacting atoms does exhibit the presence of density, or sound, waves characterizing collective phonon excitations. Any model is a cartoon of reality, and may take or not take into account the existence of phonons. But one should not confuse cartoon models and physics.

In the present paper, we show how it is possible to modify the Hubbard model in order to take into account collective phonon excitations. And we analyze the consequence of the phonon existence on the stability of insulating states. It turns out [6] that phonon excitations can strongly influence the region of stability of insulating states in optical lattices. In those cases, where the phonon instability occurs, the lattice can be metastable, and living sufficiently long time for being experimentally observed.

2. Phonon-dressed lattice model

Let us start with the general form of the Hamiltonian in the second-quantization representation,

$$\hat{H} = \int \psi^\dagger(\mathbf{r}) \left[-\frac{\nabla^2}{2m} + V_L(\mathbf{r}) \right] \psi(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \int \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \Phi(\mathbf{r}-\mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}) \, d\mathbf{r} d\mathbf{r}' \; , \tag{1}$$

in which the field operators can satisfy either Bose or Fermi statistics. The optical-lattice potential

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

is formed by laser beams with the laser wave vector

$$\mathbf{k}_0 = \left\{ k_0^\alpha = \frac{2\pi}{\lambda_\alpha} = \frac{\pi}{a_\alpha} \right\} \tag{3}$$

prescribing the lattice vector

$$\mathbf{a} = \left\{ a_\alpha = \frac{\lambda_\alpha}{2} = \frac{\pi}{k_0^\alpha} \right\} \; . \tag{4}$$

The real-space dimensionality is $d = 1, 2, 3$. The characteristic kinetic energy of an atom, caused by laser beams, is the recoil energy

$$E_R = \frac{k_0^2}{2m} \qquad \left(k_0^2 = \sum_{\alpha=1}^{d} \frac{\pi^2}{a_\alpha^2} \right) \; . \tag{5}$$

The total number of atoms N is placed inside an optical lattice, with the number of sites N_L. The lattice vectors are $\{\mathbf{a}_j : j = 1, 2, \ldots, N_L\}$. The lattice itself is fixed in space. The filling factor

$$\nu \equiv \frac{N}{N_L} = \rho a^d \tag{6}$$

can be expressed through the average atomic density ρ and mean interatomic distance a, defined as

$$\rho \equiv \frac{N}{V} \; , \qquad a^d \equiv \frac{V}{N_L} \; , \tag{7}$$

with V being the system volume.

Atomic interactions, generally, contain two parts, represented by local and nonlocal potentials

$$\Phi(\mathbf{r}) = \Phi_{loc}(\mathbf{r}) + \Phi_{non}(\mathbf{r}) \; . \tag{8}$$

The local interaction potential can be written in the form

$$\Phi_{loc}(\mathbf{r}) = \Phi_d \delta(\mathbf{r}) \; , \tag{9}$$

with the interaction strength

$$\Phi_d = \frac{\Phi_{eff}}{(\sqrt{2\pi}\, l_\perp)^{3-d}} , \qquad \Phi_{eff} \equiv 4\pi \, \frac{a_{eff}}{m} , \tag{10}$$

in which $l_\perp$ is the transverse oscillator length and a_{eff} is an effective scattering length. The latter, depending on the system geometry, takes the following values: in the quasi-one-dimensional case [7], it is

$$a_{eff} = \frac{a_s}{1 - 0.46 a_s / l_\perp} \qquad (d = 1) .$$

In the quasi-two-dimensional case [8], one has

$$a_{eff} = \frac{a_s}{1 - (a_s/\sqrt{2\pi}\, l_\perp) \ln[(2\pi)^{3/2} \rho l_\perp a_s]} \qquad (d = 2) .$$

And in three dimensions, it is just the scattering length,

$$a_{eff} = a_s \qquad (d = 3) .$$

Nonlocal interactions can correspond to dipolar forces [9, 10]

In an insulating state, atoms are localized at the points of minima of an effective potential formed by the combination of the given optical lattice and an effective potential created by other atoms. At each given moment of time the points of minima $\{\mathbf{r}_j\}$ do not necessarily coincide with the lattice sites $\{\mathbf{a}_j\}$, since atoms fluctuate. The set $\{\mathbf{r}_j\}$ of the effective minima is to be treated as a random set. As far as atoms are localized in the vicinity of the points $\{\mathbf{r}_j\}$, it is possible to expand the field operators over localized orbitals [11, 12] centered at the corresponding spatial points,

$$\psi(\mathbf{r}) = \sum_{nj} c_{nj} \psi_n(\mathbf{r} - \mathbf{r}_j) , \tag{11}$$

where n is a set of quantum numbers defining energy levels. Substituting expansion (11) into Hamiltonian (1), we consider only the lowest energy level, assuming that the gap between the energy levels is sufficiently large, being much larger than an average phonon energy. Then we obtain the Hamiltonian

$$\hat{H} = -\sum_{i \neq j} J(\mathbf{r}_{ij}) c_i^\dagger c_j + \sum_j \left(\frac{\mathbf{p}_j^2}{2m} + V_L \right) c_i^\dagger c_j + \frac{U}{2} \sum_j c_j^\dagger c_j^\dagger c_j c_j + \frac{1}{2} \sum_{i \neq j} U(\mathbf{r}_{ij}) c_i^\dagger c_j^\dagger c_j c_i , \tag{12}$$

in which $J(\mathbf{r}_{ij})$ is a hopping term, $\mathbf{p}_j^2/2m$ is a kinetic-energy term, V_L is an average of the lattice potential, U is an on-site interaction parameter, and $U(\mathbf{r}_{ij})$ describes interactions between different sites. Here $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$. The above quantities are the matrix elements over the localized orbitals, whose calculation can be found in Refs. [6, 13, 14].

Instead of the localized orbitals, it is possible to use the so-called maximally localized Wannier functions [15, 16]. These functions have been successfully employed not only for crystals with ideally periodic lattices, but also for crystals with defects, disordered networks, amorphous solids, and even liquids [15, 16]. The definition of the maximally localized Wannier functions, which can be used for the present consideration, is given in the Appendix.

Since the vector $\mathbf{r}_j$, by assumption, is a random vector, close to $\mathbf{a}_j$, it is convenient to introduce the notation

$$\mathbf{r}_j = \mathbf{a}_j + \mathbf{u}_j , \tag{13}$$

where

$$\mathbf{a}_j \equiv \langle \mathbf{r}_j \rangle , \qquad \langle \mathbf{u}_j \rangle = 0 . \tag{14}$$

Here the angle brackets mean statistical averaging with respect to the total system Hamiltonian. In a stable equilibrium state, random oscillations around the sites $\mathbf{a}_j$ imply zero average deviation $\langle \mathbf{u}_j \rangle$. A nonzero value of the latter would signify a structural phase transition [17].

For what follows, it is convenient to define the relative-distance vectors $\mathbf{a}_{ij} \equiv \mathbf{a}_i - \mathbf{a}_j$ and the relative deviations $\mathbf{u}_{ij} \equiv \mathbf{u}_i - \mathbf{u}_j$. The deviations are assumed to be small, which makes it possible to resort to the second-order expansions

$$U(\mathbf{r}_{ij}) \simeq U_{ij} + \sum_\alpha U_{ij}^\alpha u_{ij}^\alpha \; - \; \frac{1}{2} \sum_{\alpha\beta} U_{ij}^{\alpha\beta} u_{ij}^\alpha u_{ij}^\beta \; ,$$

$$J(\mathbf{r}_{ij}) \simeq J_{ij} + \sum_\alpha J_{ij}^\alpha u_{ij}^\alpha \; - \; \frac{1}{2} \sum_{\alpha\beta} J_{ij}^{\alpha\beta} u_{ij}^\alpha u_{ij}^\beta \; , \tag{15}$$

in which

$$U_{ij} \equiv U(\mathbf{a}_{ij}) \; , \qquad U_{ij}^\alpha \equiv \frac{\partial U_{ij}}{\partial a_{ij}^\alpha} = \frac{\partial U_{ij}}{\partial a_i^\alpha} \; , \qquad U_{ij}^{\alpha\beta} \equiv - \frac{\partial^2 U_{ij}}{\partial a_{ij}^\alpha \partial a_{ij}^\beta} = \frac{\partial^2 U_{ij}}{\partial a_i^\alpha \partial a_j^\beta} \; ,$$

with similar notations used for the hopping term.

Keeping in mind different physical nature of deviations and atomic operators, we employ the decoupling

$$u_{ij}^\alpha u_{ij}^\beta c_i^\dagger c_j = \langle u_{ij}^\alpha u_{ij}^\beta \rangle c_i^\dagger c_j + u_{ij}^\alpha u_{ij}^\beta \langle c_i^\dagger c_j \rangle - \langle u_{ij}^\alpha u_{ij}^\beta \rangle \langle c_i^\dagger c_j \rangle \; . \tag{16}$$

Phonon operators are introduced by the nonuniform canonical transformation [14, 18]

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

$$\mathbf{p}_j = - \frac{i}{\sqrt{2N}} \sum_{ks} \sqrt{\frac{m\omega_{ks}}{\nu}} \, \mathbf{e}_{ks} \left(b_{ks} - b_{-ks}^\dagger \right) e^{i\mathbf{k}\cdot\mathbf{a}_j} \tag{17}$$

differing from the standard transformation by the presence of the vector $\vec{\delta}_j$ that is required for cancelling in the Hamiltonian the terms linear in the phonon operators [19].

The phonon spectrum is defined by the eigenproblem

$$\frac{\nu}{m} \sum_{j(\neq i)} \sum_\beta \Phi_{ij}^{\alpha\beta} e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} e_{ks}^\beta = \omega_{ks}^2 e_{ks}^\alpha \; , \tag{18}$$

in which $\mathbf{e}_{ks}$ are the polarization vectors, s being a polarization index, and the renormalized dynamical matrix is

$$\Phi_{ij}^{\alpha\beta} = U_{ij}^{\alpha\beta} \langle c_i^\dagger c_j^\dagger c_j c_i \rangle - 2 J_{ij}^{\alpha\beta} \langle c_i^\dagger c_j \rangle \; . \tag{19}$$

In the case of a cubic lattice, it is convenient to define the effective dynamical matrix

$$D_{ij} \equiv - \frac{1}{d} \sum_{\alpha=1}^d \Phi_{ij}^{\alpha\alpha} \qquad (D_0 \equiv D_{\langle ij \rangle}) \; , \tag{20}$$

denoting the matrix in Eq. (20) for the nearest neighbour sites by D_0 .

In this way, we obtain the Hamiltonian

$$\hat{H} = E_N + \hat{H}_{at} + \hat{H}_{ph} + \hat{H}_{ind} \; , \tag{21}$$

where E_N is a non-operator quantity, the second term is the renormalized atomic Hamiltonian, the third term is the phonon Hamiltonian, and the last term describes effective atomic interactions induced by the phonon existence. Expressing these terms, we use the correlation functions

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

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

The first term reads as

$$E_N = -NK_N \; , \tag{22}$$

where K_N is the mean kinetic energy per atom

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

The atomic Hamiltonian becomes

$$\hat{H}_{at} = -\sum_{i \neq j} \widetilde{J}_{ij} c_i^{\dagger} c_j + \frac{U}{2} \sum_j c_j^{\dagger} c_j^{\dagger} c_j c_j + \frac{1}{2} \sum_{i \neq j} \widetilde{U}_{ij} c_i^{\dagger} c_j^{\dagger} c_j c_i + K_N \sum_j c_j^{\dagger} c_j \; , \tag{23}$$

with the renormalized hopping and interaction terms

$$\widetilde{J}_{ij} = J_{ij} - (1-\delta_{ij}) \sum_{\alpha\beta} J_{ij}^{\alpha\beta} \langle u_j^{\alpha} u_j^{\beta} \rangle \; , \qquad \widetilde{U}_{ij} = U_{ij} - (1-\delta_{ij}) \sum_{\alpha\beta} U_{ij}^{\alpha\beta} \langle u_j^{\alpha} u_j^{\beta} \rangle \; .$$

The phonon Hamiltonian is

$$\hat{H}_{ph} = \sum_{ks} \omega_{ks} \left(b_{ks}^{\dagger} b_{ks} + \frac{1}{2} \right) \; , \tag{24}$$

in which the phonon spectrum is defined in Eq. (18) through the renormalized dynamical matrix (19). And the induced atomic interactions result in the term

$$\hat{H}_{ind} = \sum_{i \neq j} \sum_{\alpha\beta} F_i^{\alpha} \gamma_{ij}^{\alpha\beta} F_j^{\beta} \; , \tag{25}$$

where

$$F_i^{\alpha} = \sum_{j(\neq i)} \left(2J_{ij}^{\alpha} c_i^{\dagger} c_j - U_{ij}^{\alpha} c_i^{\dagger} c_j^{\dagger} c_j c_i \right) \; , \qquad \gamma_{ij}^{\alpha\beta} = \frac{1}{N_L} \sum_{ks} \frac{e_{ks}^{\alpha} e_{ks}^{\beta}}{m\omega_{ks}^2} \; e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} \; .$$

3. Lindemann criterion of stability

An insulating state, by its definition, presupposes that atomic wave packets are well localized close to their lattice sites, so that the packets, corresponding to the nearest neighbours, practically do not overlap. As soon as the overlap becomes essential, the system cannot anymore be treated as localized. In that case, the insulating state is not stable, but there occurs the delocalization of atoms. This behavior can be discussed in terms of correlation functions: The correlation of the fluctuations in the localized state should decay exponentially on a finite correlation length ξ [20]. Then an instability due to an increasing overlap is indicated by a divergency of the correlation length. A similar description is based on the Lindemann criterion, which will be used subsequently.

The oscillations of an atomic wave packet are characterized by the mean-square deviation

$$r_0^2 \equiv \sum_{\alpha=1}^{d} \langle u_j^\alpha u_j^\alpha \rangle \; . \tag{26}$$

In an insulating state, this deviation is usually much smaller than the distance between the nearest neighbours a. The delocalization transition happens, when the mean square deviation increases approaching a. This is the Lindemann criterion of delocalization [21]. The weak form of the criterion implies that

$$\frac{r_0}{a} < 1 \; . \tag{27}$$

We calculate the mean-square deviation for a cubic lattice, with nearest-neighbour interactions, and employ the Debye approximation. The lattice is assumed to be sufficiently large, so that $N_L \gg 1$. Then, at finite temperature, we have in one dimension

$$r_0^2 \simeq \frac{T}{2\pi^2 \nu D_0} \; N_L \qquad (d = 1, \; T > 0) \; , \tag{28}$$

in two dimensions

$$r_0^2 \simeq \frac{T}{(2\pi)^2 \nu D_0} \; \ln N_L \qquad (d = 2, \; T > 0) \; , \tag{29}$$

and in three dimensions

$$r_0^2 \simeq \frac{9T}{m T_D^2} \; N_L \qquad (d = 3, \; T > T_D) \; , \tag{30}$$

where the Debye temperature is

$$T_D = \sqrt{4\pi \; \frac{\nu D_0}{m}} \; \left[\frac{d}{2} \; \Gamma\left(\frac{d}{2} \right) \right]^{1/d} \; . \tag{31}$$

This tells us that, at finite temperature, only three-dimensional insulating states can be stable.

At zero temperature, we find

$$r_0^2 = \frac{d^2}{2(d-1) m T_D} \qquad (T = 0) \; , \tag{32}$$

which shows that, at $T = 0$, two-dimensional and three-dimensional insulating states are admissible.

Summarizing, we see that insulating optical lattices can be stable with respect to collective phonon excitations: in two dimensions at zero temperature, if

$$\frac{E_R}{T_D} < \frac{\pi^2}{2} \qquad (d = 2, \; T = 0) \; , \tag{33}$$

in three dimensions at zero temperature when

$$\frac{E_R}{T_D} < \frac{2\pi^2}{3} \qquad (d = 3, \; T = 0) \; , \tag{34}$$

and in three dimensions at finite temperature, provided that

$$\frac{E_R T}{T_D^2} < \frac{\pi^2}{6} \qquad (d = 3, \; T > T_D) \; . \tag{35}$$

The meaning of these conditions is rather clear. They require that kinetic energy be smaller than potential energy by the amount in the right-hand side of these inequalities.

Even if the insulating state in an optical lattice is not stable, it can be metastable, living quite long time. The lifetime of a metastable state can be estimated by the formula

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

in which ω_0 is the effective oscillator frequency corresponding to a potential well at a lattice site, V_0 is the optical lattice barrier height, and E_R is the recoil energy. For example, in the case of a cubic optical lattice filled by ^{87}Rb atoms [22], the lifetime of the insulating state is quite long, being $t_{met} > 200$ s, which is longer than the lifetime of atoms in a trap, which allows one to accomplish the necessary measurements. The lifetime of insulating states for atoms, such as ^{52}Cr, ^{162}Er, and ^{164}Dy, possessing long-range dipole interactions [9, 10], can be even longer.

In conclusion, taking into account collective phonon degrees of freedom can essentially change the region of stability of insulating states in optical lattices [6]. The phonon instability can be characterized by the Lindemann criterion [21]. It looks that the insulating optical lattices, studied at the present time in experiments with trapped atoms, are not stable with respect to phonon excitations, but correspond to only metastable states that, although, can live sufficiently long time for being experimentally observed.

We have introduced the phonons in complete analogy with their introduction in the theory of quantum crystals [23], where, first, one considers atoms, localized in some randomly distributed spatial points close to the sites of a periodic lattice. Then, defining small deviations from these lattice sites, one introduces phonon excitations. The sole difference between the optical lattices and quantum crystals is that the lattice sites in the former are prescribed by laser beams creating the lattice, while in the case of quantum crystals, the lattice vectors have to be defined by minimizing the system free energy.

Note that sound waves exist in all interacting systems of many particles, whether in ideally periodic crystals or amorphous solids, in normal or superfluid liquids, in bulk samples or finite systems [24, 25].

Appendix: Maximally localized Wannier functions

The localized Hamiltonian (12) has been derived by employing the field-operator expansion (11) over the localized orbitals describing single-particle states of atoms localized in the vicinity of the related lattice sites. We have also mentioned that, instead of the localized orbitals, we could used the maximally localized Wannier functions [15, 16]. Here we give a brief definition of these functions in the form that would be convenient for the purpose of our paper.

Suppose, first, that atoms are localized in a lattice described by a set of lattice vectors $\{\mathbf{r}_j : j = 1, 2, \ldots, N_L\}$. Because of atomic interactions, the minima of an effective potential, defining the lattice $\{\mathbf{r}_j\}$, do not coincide with the sites of the optical lattice $\{\mathbf{a}_j\}$, although each $\mathbf{r}_j$ is close to $\mathbf{a}_j$. One can define a Bloch function

$$\varphi_{nk}(\mathbf{r}) = u_{nk}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} , \qquad u_{nk}(\mathbf{r} + \mathbf{r}_j) = u_{nk}(\mathbf{r}) .$$

However, Bloch functions are strongly nonunique, since the new function

$$\overline{\varphi}_{nk}(\mathbf{r}) = \sum U_{mn}(\mathbf{k}) \varphi_{mk}(\mathbf{r})$$

is also another Bloch function, provided that the matrix $[U_{mn}]$ is unitary, such that

$$\sum_j U^*_{jm}(\mathbf{k}) U_{jn}(\mathbf{k}) = \sum_j U_{mj}(\mathbf{k}) U^*_{nj}(\mathbf{k}) = \delta_{mn} .$$

It is straightforward to check that the new Bloch functions are orthonormal and form a complete basis,

$$\int \overline{\varphi}^{*}_{mk}(\mathbf{r})\overline{\varphi}_{np}(\mathbf{r})\, d\mathbf{r} = \delta_{mn}\delta_{kp} , \qquad \sum_{nk} \overline{\varphi}_{nk}(\mathbf{r})\overline{\varphi}^{*}_{nk}(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') .$$

Respectively, Wannier functions are also strongly nonunique, enabling the introduction of the form

$$\psi_n(\mathbf{r}-\mathbf{r}_j) \equiv \frac{1}{\sqrt{N_L}} \sum_k \overline{\varphi}_{nk}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}_j} = \frac{1}{\sqrt{N_L}} \sum_{mk} U_{mn}(\mathbf{k}) \varphi_{mk}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}_j} =$$

$$\frac{1}{\sqrt{N_L}} \sum_{mk} U_{mn}(\mathbf{k}) u_{mk}(\mathbf{r}) e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_j)} = \frac{1}{\sqrt{N_L}} \sum_{mk} U_{mn}(\mathbf{k}) u_{mk}(\mathbf{r}-\mathbf{r}_j) e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_j)} .$$

Maximally localized Wannier functions are defined as the functions, with the matrix $[U_{mn}]$ minimizing the variance functional

$$\sum_n \left(\langle r^2 \rangle_n - \langle r \rangle_n^2 \right) ,$$

where the brackets $< \cdots >_n$ imply the notation

$$\langle A(\mathbf{r}) \rangle_n \equiv \int \psi^{*}_n(\mathbf{r}) A(\mathbf{r}) \psi_n(\mathbf{r})\, d\mathbf{r} .$$

The so-defined maximally localized Wannier functions are orthogonal to each other, being strongly localized, and exponentially decaying outside of their related centers $\mathbf{r}_j$.

These well localized Wannier functions can be used for deriving the localized model (11). Then, taking into account that each location $\mathbf{r}_j$ is close to the site $\mathbf{a}_j$, small deviations are introduced as in Eqs. (13) and (14). The deviations describe atomic fluctuations corresponding to collective phonon excitations.

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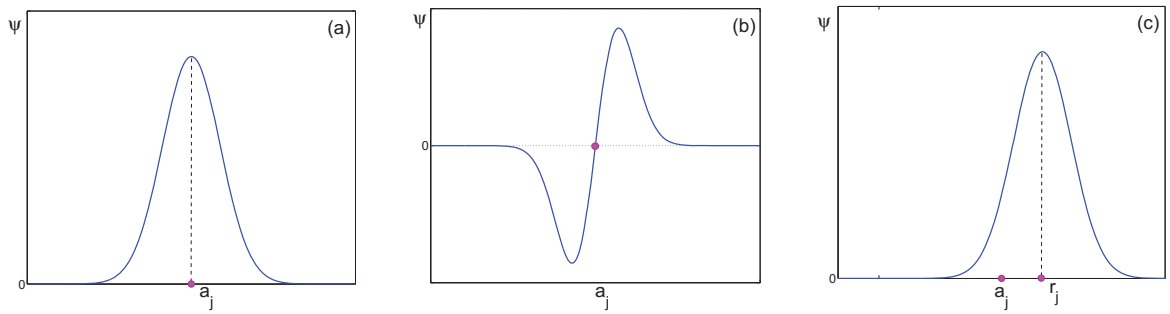

Figure 1. (a) The wave function for the ground state of an atom localized at a lattice site a_j; (b) The wave function for a localized atom in an excited single-particle state; (c) The wave function of an atom displaced from the lattice site a_j to a close position r_j, such that $|\mathbf{r}_j - \mathbf{a}_j| \ll a$, with a being the nearest neighbour lattice distance.

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