1. Introduction

Cold atoms or molecules, loaded in optical lattices, have been intensively studied both experimentally and theoretically (see, e.g. review articles [1–3] and books [4, 5]). Most often, one considers atoms or molecules weakly interacting through local potentials. Such systems are appropriately described by a single-band Hubbard model containing two constants, a tunneling parameter and on-site interaction strength. In the case of a delta-function contact interaction, atoms at different lattice sites interact very weakly and one assumes that in the majority of situations these weak interactions can be neglected. More important are long-range potentials, such as dipolar potential [5–12] making it necessary to take into account intersite interactions. But dipolar interactions also are usually treated as sufficiently weak, otherwise they can make the system unstable. In that way, the standard situation is when one treats the interaction of particles in an optical lattice as sufficiently weak, such that the single-band approximation provides an acceptable description not requiring to consider excitations above the lowest energy level. However, taking account of such collective excitations above the low-band level can essentially alter the lattice properties, for instance, rendering an insulating lattice into a conducting state [13, 14].

In the present paper, we pose and answer the general question: What happens if particle interactions in an optical lattice increase from very weak, when the system properties are mainly governed by the lattice configuration, to very strong, when the lattice potential becomes practically negligible? We show that if the interaction potential increases to such a strength, that the interactions between different lattice sites become crucial and these interactions generate collective phonon excitations, then there appears a series of three-dimensional equilibrium states, such as conducting lattices, insulating lattices, delocalized quantum crystals, and localized quantum crystals. Also, there can exist finite one- and two-dimensional lattices of chains and planes.

2. System Hamiltonian

Let us consider a system of $N$ atoms or molecules in a periodic external field formed by laser beams [15], which creates an optical lattice described by the potential

$$U_L(r) = \sum_{\alpha=1}^{d} U_\alpha \sin^2(k_0^\alpha r_\alpha),$$

in which $k_0^\alpha = 2\pi/\lambda_\alpha$. The lattice vector is defined by the laser wavelength with the components $\lambda_\alpha/2$, where $\alpha = 1, 2, \ldots, d$. 

Optical lattices are considered loaded by atoms or molecules that can exhibit strong interactions between different lattice sites. The strength of these interactions can be sufficient for generating collective phonon excitations above the ground-state energy level. Varying the interaction strength makes it possible to create several equilibrium three-dimensional phases, including conducting optical lattices, insulating optical lattices, delocalized quantum crystals, and localized quantum crystals. Also, there can exist finite one- and two-dimensional lattices of chains and planes.

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with $d$ being the space dimensionality. This potential is evid-
ently periodic with respect to the lattice vector,

$$U_L(r + r_0) = U_L(r) \quad (r'_0 = \frac{\lambda_0}{2}).$$

The single-atom lattice Hamiltonian is

$$\hat{H}_L(r) = -\frac{\nabla^2}{2m} + U_L(r).$$

The energy Hamiltonian for the system of $N$ atoms, or molecules, interacting through a potential $\Phi(r) = \Phi(-r)$, reads as

$$\hat{H} = \int \hat{\psi}^\dagger(r)\hat{H}_L(r)\hat{\psi}(r) \, dr + \frac{1}{2} \int \hat{\psi}^\dagger(r)\psi^\dagger(r') \times \Phi(r - r')\psi^\dagger(r')\hat{\psi}(r) \, dr \, dr',$$

with $\hat{\psi}$ being field operators. This Hamiltonian can also be represented in a lattice form by expanding the field operators over Wannier functions,

$$\hat{\psi}(r) = \sum_{\nu} \hat{c}_{\nu} w_{\nu}(r - r_i).$$

Here $n$ labels energy bands, while $i = 1, 2, \ldots, N_L$ enumerates lattice sites, and $r_i$ are atomic positions corresponding to an effective lattice formed by both, the optical lattice potential and by atomic interactions.

Substituting expansion (5) into Hamiltonian (4), one meets the matrix elements for the tunneling parameters

$$J_{ij}^{mn} \equiv -\int w_m^*(r - r_i)\hat{H}_L(r)w_n(r - r_i) \, dr,$$

the interaction matrix

$$U_{ij}^{mn} \equiv \int w_m^*(r - r_i)w_n^*(r' - r_j)\Phi(r - r') \times w_n(r' - r_j)w_m(r - r_i) \, dr \, dr',$$

and also the matrix elements

$$p_{mn}^2 \equiv \int w_m^*(r - r_i)(-\nabla^2)w_n(r - r_i) \, dr,$$

$$U_L^{mn} \equiv \int w_m^*(r - r_i)U_L(r)w_n(r - r_i) \, dr.$$

Then Hamiltonian (4) becomes

$$\hat{H} = -\sum_{i \neq j} \sum_{mn} J_{ij}^{mn} \hat{c}_{ni}^\dagger \hat{c}_{nj} + \sum_{mn} \left[ \frac{p_{mn}^2}{2m} + U_L^{mn} \right] \hat{c}_{ni}^\dagger \hat{c}_{nj} + \frac{1}{2} \sum_{\{i, j\}} U_{ij}^{mn} \hat{c}_{ni}^\dagger \hat{c}_{nj} \hat{c}_{nj}^\dagger \hat{c}_{ni}.$$

Unifying these limiting situations. For this purpose, it is possible to resort to the description employed for quantum crystals by combining a self-consistent approach characterizing a low-energy level above which there appear collective phonon excitations [16, 17]. It is also always possible to choose well-localized Wannier functions [18], such that the nondiagonal term $U_{iij}$ be much smaller than the diagonal $U_{iij}$. For a single band, Hamiltonian (9) reduces to the form

$$\hat{H} = -\sum_{i \neq j} J_{ij} \hat{c}_i^\dagger \hat{c}_j + \sum_{j} \left[ \frac{p_j^2}{2m} + U_L \right] \hat{c}_j^\dagger \hat{c}_j$$

$$+ \frac{1}{2} \sum_{i \neq j} U_{ij} \hat{c}_i^\dagger \hat{c}_j \hat{c}_j^\dagger \hat{c}_i,$$

in which

$$J_{ij} = -\int w^*(r - r_i)\hat{H}_L(r)w(r - r_j) \, dr \quad (i \neq j),$$

$$U_{ij} = \int |w(r - r_i)|^2 \Phi(r - r') |w(r' - r_j)|^2 \, dr \, dr',$$

$$p_j^2 = \int w^*(r - r_j)(-\nabla^2)w(r - r_j) \, dr,$$

$$U_L = \int |w(r)|^2 U_L(r) \, dr.$$ This Hamiltonian corresponds to the Hubbard model, if we omit the terms with $p_j^2$, $U_L$, and with the intersite interactions $U_{ij}$. But these terms are necessary for considering collective phonon excitations.

3. Low-energy states

Low-energy states of a many-body system in a periodic potential can be described by using Green function approach. Here we follow the method suggested in [19–21].

We consider the grand Hamiltonian

$$H = \hat{H} - \mu \int \hat{\psi}^\dagger(r)\hat{\psi}(r) \, dr,$$

with a chemical potential $\mu$. Green functions are defined as the propagators [22]

$$G(r, t, r', t') \equiv -i\langle T\hat{\psi}(r, t)\hat{\psi}^\dagger(r', t) \rangle,$$

where $T$ is a time-ordering operator and the angle brackets imply statistical averaging. Green functions satisfy the Dyson equation that in the matrix form can be written as

$$G = G_0 + G_0 \left( \Sigma - \Sigma_0 \right) G,$$

with $\Sigma$ being the self-energy and $G_0$ and $\Sigma_0$ being a Green function and self-energy of a trial approximation.

For an equilibrium system, the Green functions depend on time difference,

$$G(r, t, r', t') = G(r, r', t - t'),$$

(15)
allowing us to define the Fourier transform
\[ G(r, r', \omega) = \int_{-\infty}^{\infty} G(r, r', t) e^{i\omega t} \, dt . \] (16)

Then the Dyson equation (14) writes as
\[ G(r, r', \omega) = G_0(r, r', \omega) + \int K(r, r'', \omega) G(r'', r', \omega) \, dr'' , \] (17)
with the kernel
\[ K(r, r', \omega) = \int G_0(r, r'', \omega) [ \Sigma(r'', \omega) - \Sigma_0(r'', \omega) ] \, dr''. \] (18)

Equation (17) can be solved by means of an iterative procedure starting with the initial approximation \( G_0 \). Thus the first-order iteration yields
\[ G_1(r, r', \omega) = G_0(r, r', \omega) + \int K_1(r, r'', \omega) G_0(r'', r', \omega) \, dr'' , \] (19)
with the kernel
\[ K_1(r, r', \omega) = \int G_0(r, r'', \omega) [ \Sigma_1(r'', \omega) - \Sigma_0(r'', \omega) ] \, dr''. \] (20)

For the self-energy of zero approximation, it is possible to take the diagonal form
\[ \Sigma_0(r, r', \omega) = U_0(r) \delta(r-r') , \] (21)
with a trial potential that is periodic over the lattice vectors,
\[ U_0(r + \mathbf{r}_j) = U_0(r) . \] (22)

Then the first-order self-energy reads as
\[ \Sigma_1(r, r', \omega) = \delta(r-r') \left[ U_1(r) + \int \Phi(r-r'') \rho(r'') \, dr'' \right] , \] (23)
where the atomic density is
\[ \rho(r) = \langle \hat{\psi}^\dagger(r) \hat{\psi}(r) \rangle = \pm i \lim_{\tau \to +0} \int_{-\infty}^{\infty} e^{i\omega \tau} G(r, r', \omega) \frac{d\omega}{2\pi} . \] (24)

Here the upper sign corresponds to bosons, while the lower, to fermions. The kernel (20) becomes
\[ K_1(r, r', \omega) = G_0(r, r', \omega) \left[ U_1(r) - U_0(r) \right] , \] (25)
with the effective potential
\[ U_1(r) = U_L(r) + \int \Phi(r-r') \rho_0(r') \, dr' . \] (26)

The Green function, corresponding to self-energy (21) can be represented as the expansion over Wannier functions
\[ G_0(r, r', \omega) = \sum_{mn} G_n(\omega) w_n(r-r_j) w_{n'}^*(r'-r_j) , \] (27)
where
\[ G_n(\omega) = \frac{1 \pm n(\omega_n)}{\omega - \omega_n + i0} = \frac{n(\omega_n)}{\omega - \omega_n + i0} . \] (28)

and
\[ n(\omega) = \left( e^{\beta \omega} + 1 \right)^{-1} \left( \beta \equiv \frac{1}{T} \right) . \]

The frequency \( \omega_n = E_n - \mu \) characterizes the energy \( E_n \) of the \( n \)th quantum state, shifted by the chemical potential. The related zero-order approximation for the atomic density is
\[ \rho_0(r) = \sum_{nj} n(\omega_n) \left| w_n(r-r_j) \right|^2 . \] (29)

In that way, the first-order Green function acquires the form
\[ G_1(r, r', \omega) = G_0(r, r', \omega) + \int \sum_{mn} G_m(\omega) G_n(\omega) \Delta_{nj}^{mn} w_m(r-r_j) w_n^*(r'-r_j) \, dr, \] (30)

in which
\[ \Delta_{nj}^{mn} = \int w_n^*(r-r_j) \left[ U_1(r) - U_0(r) \right] w_m(r-r_j) \, dr . \] (31)

The choice of the trial potential (22) is not arbitrary but has to be defined in such a way that to induce the convergence of the iterative procedure. This can be done by employing optimized perturbation theory [19–21, 23]. For this purpose, it is possible to require that the sequence of approximations for observable quantities \( \langle \hat{A} \rangle_k \), related to the operator \( \hat{A} \), be convergent. As a self-consistency condition, optimizing the choice, one can take
\[ \langle \hat{A} \rangle_{k+1} - \langle \hat{A} \rangle_k = 0 . \] (32)

For an operator of the form
\[ \hat{A} = \int \hat{\psi}^\dagger(r) \hat{A}(r) \hat{\psi}(r) \, dr , \] (33)
the \( k \)th order approximation is
\[ \langle \hat{A} \rangle_k = \pm i \lim_{\tau \to +0} \int_{-\infty}^{\infty} e^{i\omega \tau} \lim_{\tau \to -0} \hat{A}(r') G_k(r, r', \omega) \, dr \frac{d\omega}{2\pi} . \] (34)

Then the optimization condition
\[ \langle \hat{A} \rangle_1 - \langle \hat{A} \rangle_0 = 0 \] (35)
results in the equation
\[ \sum_{mn} \sum_{ij} n(\omega_m) - n(\omega_n) \Delta_{nj}^{mn} A_{ij}^{mn} = 0 . \] (36)

The main contribution into sum (36) is brought by the diagonal terms, which allows us to write
\[ \sum_{nj} n(\omega_n) [ 1 \pm n(\omega_n) ] \Delta_{nj}^{mn} A_{ij}^{mn} = 0 . \] (37)

In the single-band picture, considering only the lowest band, we get
\[ \Delta_{jj}^{00} = 0 . \] (38)
Explicitly, the latter equation writes as
\[ 
\int |w(r - r_j)|^2 U_0(r) \, dr = \int |w(r - r_j)|^2 U_L(r) \, dr 
\]  
\[ 
+ \int |w(r - r_j)|^2 \Phi(r - r') \rho_0(r') \, dr \, dr' \, , 
\]  
with the atomic density
\[ 
\rho_0(r) = \sum_j \nu \left| w(r - r_j) \right|^2 
\]  
and the filling factor
\[ 
\nu \equiv \frac{N}{N_L} = \sum_n n(\omega_n) \, . 
\]

Taking into account the periodicity of the potentials \( U_0 \) and \( U_L \) leads to the condition
\[ 
\int |w(r)|^2 U_0(r) \, dr = \int |w(r)|^2 U_L(r) \, dr 
\]  
\[ 
+ \int |w(r)|^2 \Phi(r - r') \rho_0(r') \, dr \, dr' \, . 
\]  

Thus when the optimization condition (38), or (42), is valid, the Green functions of zero and first order and, respectively, observable quantities of zero and first order are close to each other.

4. Trial potential

The optimization condition (42) imposes a constraint on the choice of the trial potential \( U_0 \). For instance, in the vicinity of \( r \sim 0 \), one can accept the potential of the form
\[ 
U_0(r) \simeq u_0 + \sum_{\alpha=1}^d \frac{m}{2} \varepsilon_\alpha r_\alpha^2 \, , 
\]  
where \( u_0 \) is a static field and \( \varepsilon_\alpha \) are effective frequencies of atomic oscillations. The related zero-order Wannier function can be approximated by the harmonic expression
\[ 
w_n(r) = \prod_\alpha \left( \frac{m \varepsilon_\alpha / \pi}{2^{\alpha_n} n_\alpha!} \right)^{1/4} H_{\alpha_n} \left( \frac{r_\alpha}{l_\alpha} \right) \exp \left( -\frac{r_\alpha^2}{2 l_\alpha^2} \right) \, , 
\]  
in which \( n_\alpha = 0, 1, 2, \ldots \) and
\[ 
l_\alpha \equiv \frac{1}{\sqrt{m \varepsilon_\alpha}} \, . 
\]
The lowest-energy function (44) is
\[ 
w(r) = \prod_\alpha \left( \frac{m \varepsilon_\alpha / \pi}{2^{\alpha_n} n_\alpha!} \right)^{1/4} \exp \left( -\frac{r_\alpha^2}{2 l_\alpha^2} \right) \, . 
\]

In the vicinity of \( r \sim 0 \), the optical-lattice potential can be written as
\[ 
U_L(r) \simeq \sum_{\alpha=1}^d \frac{m}{2} \omega_\alpha^2 r_\alpha^2 \quad (r_\alpha \rightarrow 0) \, . 
\]  
with the frequency
\[ 
\omega_\alpha \equiv \frac{2\pi}{l_\alpha} \sqrt{\frac{2}{m} U_\alpha} \, . 
\]  

Introducing the recoil energy
\[ 
E_R^\alpha \equiv \frac{\hbar^2}{2 m l_\alpha^2} \, , 
\]  
for the optical-lattice frequency (47), we have
\[ 
\omega_\alpha = 2 \sqrt{E_R^\alpha U_\alpha} \, . 
\]

Setting the static field
\[ 
u_0 = \nu \sum_j \Phi(r_j) \]

yields the equation for the effective trial frequency \( \varepsilon_\alpha \),
\[ 
\frac{1}{4} \sum_\alpha \left( \varepsilon_\alpha - \omega_\alpha^2 \nu_0 - \Omega_\alpha^2 \right) = 0 \, , 
\]  
in which
\[ 
\Omega_\alpha^2 \equiv \frac{2\nu}{m} \sum_j \frac{\partial^2 \Phi(r_j)}{\partial r_{\alpha j}^2} \, . 
\]

Then we find the effective trial frequency
\[ 
\varepsilon_\alpha = \sqrt{\omega_\alpha^2 + \Omega_\alpha^2} \, . 
\]

The meaning of the formula (54) is rather clear. The effective oscillation frequency of atoms is defined by the optical-lattice potential as well as by atomic interactions. If the interactions are absent, the frequency is completely prescribed by the optical-lattice potential,
\[ 
\varepsilon_\alpha = \omega_\alpha \quad (\Omega_\alpha = 0) \, . 
\]

When the interactions are not zero, but yet rather weak, the effective frequency is close to that defined by the optical lattice, with small corrections caused by the interactions,
\[ 
\varepsilon_\alpha \simeq \omega_\alpha \left( 1 + \frac{\Omega_\alpha^2}{2 \omega_\alpha^2} \right) \quad (\Omega_\alpha \ll \omega_\alpha) \, . 
\]

But when the interactions are strong, the effective oscillation frequency is mainly governed by atomic interactions, while the optical lattice provides small corrections,
\( \varepsilon_{\alpha} \simeq \Omega_{\alpha} \left( 1 + \frac{\omega_{\alpha}^2}{2 \Omega_{\alpha}^2} \right) \quad (\omega_{\alpha} \ll \Omega_{\alpha}) . \)  

(57)

And if the interactions are so strong that the optical lattice becomes negligible, the oscillations are caused by atomic interactions,

\[ \varepsilon_{\alpha} = \Omega_{\alpha} \quad (\omega_{\alpha} = 0) . \]

(58)

In the intermediate case, both the optical lattice as well as atomic interactions, regulate the effective frequency of atomic motion.

### 5. Energy levels

The energy levels for a many-body system can be defined in the following way. The equation of motion for Green functions can be written as

\[ \int G^{-1}(r, r', \omega)G(r'', r', \omega) \, dr'' = \delta(r - r') , \]

(59)

where the inverse propagator is

\[ G^{-1}(r, r', \omega) = (\omega + \mu)\delta(r - r') - H(r, r', \omega) , \]

(60)

with the effective Hamiltonian kernel

\[ H(r, r', \omega) = -\frac{\nabla^2}{2m} \delta(r - r') + \Sigma(r, r', \omega) . \]

(61)

Introducing the effective Hamiltonian acting on Green functions by the formula

\[ \hat{H}(r, \omega)G(r, r', \omega) = \int \hat{H}(r, r'', \omega)G(r'', r', \omega) \, dr'' , \]

(62)

we come to the equation

\[ [\omega + \mu - \hat{H}(r, \omega)]G(r, r', \omega) = \delta(r - r') . \]

(63)

When there exists a solution for the eigenproblem

\[ \hat{H}(r, \omega)\varphi_n(r) = E_n\varphi_n(r) , \]

(64)

then and only then the Green function can be represented as the expansion

\[ G(r, r', \omega) = \sum_n G_n(\omega)\varphi_n(r)\varphi^*_n(r') , \]

(65)

in which \( G_n(\omega) \) is given by equation (28). Equation (64), called the effective Schrödinger equation, defines the energy levels of a many-body system. The energy eigenvalues \( E_n \) can be found by resorting to optimized perturbation theory [23].

The zero approximation can be modeled by a diagonal Hamiltonian kernel

\[ H_0(r, r', \omega) = \hat{H}_0(r)\delta(r - r') , \]

(66)

with the Hamiltonian

\[ \hat{H}_0(r) = -\frac{\nabla^2}{2m} + U_0(r) \]

(67)

that is periodic over the lattice vectors

\[ \hat{H}_0(r + r_j) = \hat{H}_0(r) . \]

However, Wannier functions are not eigenfunctions of this Hamiltonian (67). The eigenfunctions of a periodic Hamiltonian are Bloch functions,

\[ \hat{H}_0(r)\varphi_{nk}(r) = E_{nk}\varphi_{nk}(r) . \]

Expressing the Bloch functions through Wannier functions,

\[ \varphi_{nk}(r) = \frac{1}{\sqrt{N_L}} \sum_j w_n(r - r_j)e^{ikr_j} , \]

where we see that the action of the Hamiltonian on a Wannier function gives

\[ \hat{H}_0(r)w_n(r - r_j) = \sum_i E_{ij}^n w_n(r - r_i) . \]

(68)

Equation (68) can be transformed into

\[ \hat{H}_0(r)\psi_n(r) = E_n\psi_n(r) , \]

(69)

with

\[ \psi_n(r) = \sum_j w_n(r - r_j) , \quad E_n = \sum_j E_{ij}^n . \]

Hence the eigenfunctions of \( \hat{H}_0 \) are either Bloch functions or the sums \( \psi_n(r) \) of Wannier functions.

But in the vicinity of \( r \approx r_j \) equation (69) takes the form

\[ \hat{H}_0(r)w_n(r - r_j) = E_n w_n(r - r_j) , \]

(70)

which means that Wannier functions are approximate solutions of this equation, in which \( n = \{n_\alpha\} \) and \( n_\alpha = 0, 1, 2, \ldots \).

We accept the trial potential (43), where the quantities \( \varepsilon_\alpha \) play the role of control functions. Then the zero-order energy levels are

\[ E_n^{(0)} = u_0 + \sum_\alpha \left(n_\alpha + \frac{1}{2}\right)\varepsilon_\alpha . \]

(71)

In the first order, equation (64) yields the eigenvalues

\[ E_n^{(1)} = \int \psi_n^*(r)\hat{H}_1(r)\psi_n(r) \, dr , \]

(72)

where

\[ \hat{H}_n^{(1)} = -\frac{\nabla^2}{2m} + U_1(r) \]

(73)

and \( U_1(r) \) is defined by equation (26).

Considering only the ground-state energy level, we have the zero-order eigenvalue

\[ E_0^{(0)} = u_0 + \frac{1}{2} \sum_\alpha \varepsilon_\alpha . \]

(74)
Since
\[ \int w(r) \left( -\frac{\nabla^2}{2m} \right) w(r) \, dr = \frac{1}{4} \sum_\alpha \varepsilon_\alpha , \]
for the first-order approximation, we get
\[ E_0^{(1)} = \frac{1}{4} \sum_\alpha \varepsilon_\alpha + \int |w(r)|^2 U_1(r) \, dr . \quad (75) \]
From here, we find
\[ E_0^{(1)} = u_0 + \frac{1}{4} \sum_\alpha \left( \varepsilon_\alpha + \frac{\omega^2}{\varepsilon_\alpha} + \frac{\Omega^2}{\varepsilon_\alpha} \right) . \quad (76) \]
The trial frequency \( \varepsilon_\alpha \) can be defined by the optimization condition
\[ E_0^{(1)} - E_0^{(0)} = 0 , \quad (77) \]
which results in the same expression (54) for the frequency \( \varepsilon_\alpha \).

6. Collective excitations

In the previous sections, we have described the lowest energy state of an atomic system. This is actually the system ground state that is formed by an ensemble of atoms represented by harmonic oscillators, with a self-consistently defined frequency taking into account the presence of both, an optical lattice as well as of intersite atomic interactions. Collective excitations in such a system are known to be phonons [16, 24–26] that can be introduced in the following way.

One treats the vectors \( \mathbf{r}_i \) as the operators having the form
\[ \mathbf{r}_i = \mathbf{a}_i + \mathbf{u}_i , \quad (78) \]
where \( \mathbf{a}_i \) is a vector of an absolutely equilibrium effective lattice, while \( \mathbf{u}_i \) is a deviation operator, so that
\[ \mathbf{a}_i \equiv \langle \mathbf{r}_i \rangle , \quad \langle \mathbf{u}_i \rangle = 0 . \quad (79) \]
Also, it is convenient to introduce the relative quantities
\[ \mathbf{r}_i \equiv \mathbf{r}_i - \mathbf{r}_j = \mathbf{a}_i - \mathbf{u}_i , \quad \mathbf{a}_i = \mathbf{a}_i - \mathbf{a}_j , \quad \mathbf{u}_i = \mathbf{u}_i - \mathbf{u}_j . \]

In the representation (10) of the system Hamiltonian, one has
\[ J_y = J(\mathbf{r}_y) , \quad U_y = U(\mathbf{r}_y) , \quad U_y = U(0) \equiv U . \quad (80) \]
These quantities are expanded in powers of the deviations from the lattice sites \( \mathbf{a}_i \), keeping the terms up to the second order,
\[ J(\mathbf{r}_y) \simeq J(\mathbf{a}_y) + \sum_\alpha J_{y\alpha}^{\alpha} a_\alpha + \frac{1}{2} \sum_\alpha J_{y\alpha}^{\alpha\beta} a_\alpha a_\beta , \]
\[ U(\mathbf{r}_y) \simeq U(\mathbf{a}_y) + \sum_\alpha U_{y\alpha}^{\alpha} a_\alpha + \frac{1}{2} \sum_\alpha U_{y\alpha}^{\alpha\beta} a_\alpha a_\beta . \quad (81) \]

using the notations
\[ J_{y\alpha}^{\alpha} \equiv \frac{\partial J(\mathbf{a}_\alpha)}{\partial a_\alpha} = \frac{\partial J(\mathbf{a}_\alpha)}{\partial a_\alpha} , \quad U_{y\alpha}^{\alpha} \equiv \frac{\partial U(\mathbf{a}_\alpha)}{\partial a_\alpha} = \frac{\partial U(\mathbf{a}_\alpha)}{\partial a_\alpha} . \]

Vibrational and atomic degrees of freedom can be decoupled according to the rule
\[ a_\alpha^{\dagger} a_\alpha^{\dagger} \tilde{c}_i \tilde{c}_j = \langle a_\alpha^{\dagger} a_\alpha^{\dagger} \tilde{c}_i \tilde{c}_j \rangle + a_\alpha^{\dagger} a_\alpha^{\dagger} (\tilde{c}_i \tilde{c}_j) - \langle a_\alpha^{\dagger} a_\alpha^{\dagger} \rangle \langle \tilde{c}_i \tilde{c}_j \rangle . \quad (82) \]

Then one can define the renormalized tunneling parameter
\[ \tilde{J}_{ij} \equiv J(\mathbf{a}_j) - \frac{1}{2} \sum_{\alpha\beta} J_{ij}^{\alpha\beta} (a_\alpha^0 a_\beta^0) , \quad (83) \]
renormalized atomic interactions
\[ \tilde{U}_{ij} \equiv U(\mathbf{a}_j) - \frac{1}{2} \sum_{\alpha\beta} U_{ij}^{\alpha\beta} (a_\alpha^0 a_\beta^0) , \quad (84) \]
renormalized dynamic interactions
\[ \Phi_{ij}^{\alpha\beta} \equiv U_{ij}^{\alpha\beta} \langle \tilde{c}_i \tilde{c}_j \rangle - 2J_{ij}^{\alpha\beta} \langle \tilde{c}_i \tilde{c}_j \rangle . \quad (85) \]

and the effective force
\[ F_{ij}^{\alpha} = 2J_{ij}^{\alpha\beta} \langle \tilde{c}_i \rangle - U_{ij}^{\alpha\beta} \langle \tilde{c}_i \rangle . \quad (86) \]
The filling factor (41) becomes
\[ \nu \equiv \frac{N}{N_L} = \frac{1}{N_L} \sum_j \langle \tilde{c}_j \rangle = \langle \tilde{c}_j \rangle . \quad (87) \]
In that way, we come to the Hamiltonian
\[ \hat{H} = \hat{H}_N + \hat{H}_{at} + \hat{H}_{cob} + \hat{H}_{def} . \quad (88) \]
The first is the nonoperator term
\[ E_N = \frac{1}{4} \sum_{i \neq j} \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} (a_\alpha^0 a_\beta^0) - \nu \sum_j \left( \frac{\mathbf{p}_j^2}{2m} \right) . \quad (89) \]
The second is the renormalized atomic term
\[ \hat{H}_{at} = - \sum_{i \neq j} \tilde{J}_{ij} \tilde{c}_i \tilde{c}_j + \frac{U}{2} \sum_j \tilde{c}_j \tilde{c}_j + \frac{1}{2} \sum_{i \neq j} \tilde{U}_{ij} \tilde{c}_i \tilde{c}_j + \sum_j \left( \frac{\mathbf{p}_j^2}{2m} + U_L \right) \tilde{c}_j \tilde{c}_j . \quad (90) \]
The third is the term with vibrational degrees of freedom

$$\hat{H}_{vib} = \nu \sum_j \frac{p_j^2}{2m} + \frac{1}{4} \sum_{ij} \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} u_i^\alpha u_j^\beta. \quad (91)$$

Substituting here $a_j^\dagger = a_i - a_j$ yields

$$\hat{H}_{vib} = \nu \sum_j \frac{p_j^2}{2m} + \frac{1}{4} \sum_{ij} \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} u_i^\alpha u_j^\beta. \quad (92)$$

And the last term

$$\hat{H}_{def} = -\frac{1}{2} \sum_{ij} \sum_{\alpha} F_{ij}^\alpha u_i^\alpha u_j^\alpha \quad (93)$$
describes local deformations of the lattice. Introducing the notation for the effective force acting on a $j$th atom

$$F_j^\alpha = \sum_{i \neq j} F_{ij}^\alpha, \quad (94)$$

with the properties

$$F_j^\alpha = -(F_j^\alpha)^+, \quad (F_j^\alpha)^+ = 0, \quad (95)$$

we obtain

$$\hat{H}_{def} = -\frac{1}{2} \sum_j \sum_{\alpha} \left[ F_j^\alpha + (F_j^\alpha)^+ \right] u_j^\alpha. \quad (96)$$

Following the method of decoupling of atomic and vibrational degrees of freedom, we have

$$F_j^\alpha u_j^\alpha = F_j^\alpha (u_j^\alpha)^+ + (F_j^\alpha)^+ u_j^\alpha - (F_j^\alpha) (u_j^\alpha)^+. \quad (97)$$

But, since $(F_j^\alpha)^+ = 0$ and $(u_j^\alpha)^+ = 0$, we come to the conclusion that the deformation term is negligible, $H_{def} = 0$.

At the next step, we introduce phonon operators $b_{ks}$ by the canonical transformation

$$u_j = \delta_j^s + \frac{1}{\sqrt{2N}} \sum_k \sqrt{\frac{\nu}{m \omega_k}} e_{ks} \left( b_k + b_k^\dagger \right) e^{i k a_j},$$

$$p_j = -\frac{i}{\sqrt{2N}} \sum_k \sqrt{\frac{m \omega_k}{\nu}} e_{ks} \left( b_k - b_k^\dagger \right) e^{i k a_j}, \quad (98)$$
in which $k$ is momentum, $s$ is a polarization label, $e_{ks}$ are the polarization vectors with the properties

$$e_{ks} = e_{-ks}, \quad \sum_s e_{ks}^\dagger e_{ks} = \delta_{\alpha\beta}, \quad e_{ks} \cdot e_{ks'} = \sum_{\alpha} e_{ks\alpha} e_{ks'\beta} = \delta_{\alpha\beta},$$

and the phonon spectrum $\omega_k = \omega_{-k}$ is defined by the eigenproblem

$$\frac{\nu}{m} \sum_{k \neq \{\neq j\}} \sum_{\beta} \delta_{ij}^\alpha e_{k\beta} a_j^\beta e_{ks} = \omega_k^2 e_{ks}, \quad (99)$$

The first term in the first of equation (98) is responsible for the diagonalization of the phonon Hamiltonian, if the deformation part is taken into account, which requires the equality

$$\delta_{ij}^\alpha = \sum_{\beta} \gamma_{ij}^{\alpha\beta} F_i^\beta, \quad (\text{with}) \quad \gamma_{ij}^{\alpha\beta} \equiv \frac{\nu}{m} \sum_{k \neq j} e_{ks\alpha} e_{k\beta} e^{i k a_j}. \quad (100)$$

On the average,

$$\langle \delta_{ij}^\alpha \rangle = 0 .$$

Thus Hamiltonian (88) is transformed into

$$\hat{H} = E_N + \hat{H}_{at} + \hat{H}_{ph} + \hat{H}_{ind}, \quad (100)$$

where $E_N$ and $\hat{H}_{at}$ are given by equations (89) and (90). The phonon Hamiltonian is

$$\hat{H}_{ph} = \sum_k \omega_k \left( b_k^\dagger b_k + \frac{1}{2} \right), \quad (101)$$

and the term

$$\hat{H}_{ind} = \sum_{k \neq j} \sum_{\alpha\beta} F_{ij}^\alpha \gamma_{ij}^{\alpha\beta} F_j^\beta \quad (102)$$

characterizes additional atomic interactions induced by local deformations caused by phonon exchange. This term does not arise, if the deformation Hamiltonian (96) has been neglected, as is explained above. The induced term (102) also is zero, if we involve the decoupling

$$F_i^\alpha F_j^\beta = F_i^\alpha (F_j^\beta) + (F_i^\alpha) F_j^\beta - (F_i^\alpha) (F_j^\beta) \equiv 0, \quad \langle F_i^\alpha \rangle = 0.$$ 

7. Average quantities

In this way, the atomic system, including collective phonon excitations, is described by the Hamiltonian

$$\hat{H} = E_N + \hat{H}_{at} + \hat{H}_{ph}, \quad (103)$$
in which the atomic and phonon degrees of freedom are separated. Respectively, the Hilbert space of the system is represented by the tensor product

$$\mathcal{H} = \mathcal{H}_{at} \otimes \mathcal{H}_{ph}, \quad (104)$$
of the Hilbert spaces corresponding to atomic and phonon degrees of freedom. Then the partition function takes the form

$$\text{Tr}_{\mathcal{H}_e} e^{-\beta \hat{H}} = e^{-\beta E_N} \text{Tr}_{\mathcal{H}_{at}} e^{-\beta \hat{H}_{at}} \text{Tr}_{\mathcal{H}_{ph}} e^{-\beta \hat{H}_{ph}}. \quad (105)$$

The averages of the operators, acting on either the atomic Hilbert space or on the phonon Hilbert space, are calculated according to the rule

$$\langle \hat{A}_{at} \rangle = \frac{\text{Tr}_{\mathcal{H}_e} \hat{A}_{at} e^{-\beta \hat{H}}}{\text{Tr}_{\mathcal{H}_e} e^{-\beta \hat{H}}}, \quad (106)$$

$$\langle \hat{A}_{ph} \rangle = \frac{\text{Tr}_{\mathcal{H}_e} \hat{A}_{ph} e^{-\beta \hat{H}}}{\text{Tr}_{\mathcal{H}_e} e^{-\beta \hat{H}}}. \quad (106)$$
Thus we find the averages
\[
\langle u_y^t u_y^r \rangle = 2(1 - \delta_{ij}) \langle u_y^t u_y^r \rangle ,
\]
\[
\langle u_x^t u_y^r \rangle = \delta_{ij} \frac{\nu}{2N} \sum_{ks} \epsilon_k^x \epsilon_k^y \text{coth} \left( \frac{\omega_k}{2T} \right) ,
\]
\[
\left( \frac{\mathbf{p}}{2m} \right)^2 = \frac{1}{4\nu/N} \sum_{ks} \omega_k \text{coth} \left( \frac{\omega_k}{2T} \right) ,
\]
where the phonon frequency is given by the expression
\[
\omega_k^2 = \frac{\nu}{m} \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} \epsilon_k^\alpha \epsilon_k^\beta \text{e}^{\mathbf{i} \mathbf{a}_i^k} .
\]

An important quantity characterizing the atomic localization is the mean square deviation
\[
\langle u_x^t u_y^r \rangle = \epsilon_{ij} \frac{\nu}{2d} .
\]

In conclusion to this section, let us show how the parametrization of the atomic localization is related to the mean square deviation. To be more concrete, we shall use the Debye approximation that is known to be a good description of quantum lattice structures [16] and optical lattices [26].

8. Mean square deviation

The mean square deviation (109) is an important quantity characterizing the stability of localized states. To be more concrete, we shall use the Debye approximation that is known to be a good description of quantum lattice structures [16] and optical lattices [26].

Defining the effective average frequency by the equation
\[
\omega_k^2 = \frac{1}{d} \sum_{i=1}^d \omega_{ks}^2 ,
\]
we get
\[
\omega_k^2 = -\frac{\nu}{m} \sum_{j(\neq i)} D_{ij} \text{e}^{\mathbf{k} \mathbf{a}_i^j} ,
\]
with the dynamical matrix
\[
D_{ij} = -\frac{1}{d} \sum_{\alpha=1}^d \Phi_{ij}^{\alpha\alpha} \quad (i \neq j) .
\]
Keeping in mind that atoms are well localized in their lattice sites means that \( \hat{c}_i^\dagger \hat{c}_i^\prime = \nu \delta_{ij} \). Then we have
\[
\Phi_{ij}^{\alpha\beta} = \nu^2 U_{ij}^{\alpha\beta} = \nu^2 \frac{\partial^2 U(a_{ij})}{\partial a_i^\alpha \partial a_j^\beta} ,
\]
which gives the dynamical matrix
\[
D_{ij} = -\frac{\nu}{m} \sum_{\alpha=1}^d \frac{\partial^2 U(a_{ij})}{\partial a_i^\alpha \partial a_j^\alpha} = \frac{\nu}{d} \sum_{\alpha=1}^d \frac{\partial^2 U(a_{ij})}{\partial a_i^\alpha \partial a_j^\alpha} .
\]
In this approximation, the mean square deviation (109) becomes
\[
\langle u_x^t u_y^r \rangle = \nu d \frac{1}{2m \rho} \int_0^{2\pi} dk \text{coth} \left( \frac{\omega_k}{2T} \right) \frac{d^k}{(2\pi)^d} ,
\]
with the integration over the Brillouin zone.

Taking, for concreteness, a cubic lattice with the nearest-neighbour distance \( a \), we have for the frequency (116) the expression
\[
\omega_k^2 = \frac{4\nu}{m} \sum_{\alpha=1}^d \sin^2 \left( \frac{k_\alpha a}{2} \right) ,
\]
where the dynamic parameter is
\[
D = \frac{\nu}{d} \sum_{\alpha=1}^d \frac{\partial^2 U(a)}{\partial a_i^\alpha \partial a_j^\alpha} .
\]
In the long-wave limit, the spectrum is of the phonon type,
\[
\omega_k \simeq c_0 k \left( k^2 = \frac{d}{\pi c_0^2} \to 0 \right) ,
\]
with the sound velocity
\[
c_0 = \sqrt{\frac{\nu}{m} Da^2} .
\]
In the Debye approximation, one replaces the integration over the Brillouin zone by the integration over the Debye sphere, so that
\[
\int_B \frac{dk}{(2\pi)^d} \rightarrow \frac{2}{(4\pi)^{d/2}} \int_0^{k_D} k^{d-1} dk.
\] (125)

The Debye radius \(k_D\) is found from the normalization
\[
\int_B \frac{dk}{(2\pi)^d} = \frac{N_k}{V} = \frac{\rho}{\nu},
\] (126)
in which \(\rho\) is average density
\[
\rho = \frac{N}{V} = \frac{\nu}{a^d}.
\] (127)

This gives the Debye radius
\[
k_D = \frac{\sqrt{\pi d}}{a} \left[ \frac{d}{2} \Gamma \left( \frac{d}{2} \right) \right]^{1/d}.
\] (128)

For particular dimensionalities, we have
\[
k_D = \frac{\pi}{a} \quad (d = 1),
\]
\[
k_D = \frac{2\sqrt{\pi}}{a} \quad (d = 2),
\]
\[
k_D = \frac{(6\pi^2)^{1/3}}{a} \quad (d = 3).
\] (129)

One accepts the phonon spectrum (123),
\[
\omega_k = c_0 k \quad (0 \leq k \leq k_D)
\] (130)
that is cut from above by the Debye temperature
\[
T_D = c_0 k_D = \sqrt{4\pi m d \left[ \frac{d}{2} \Gamma \left( \frac{d}{2} \right) \right]^{1/d}}.
\] (131)

Thus for different dimensionalities, one has
\[
T_D = \frac{\pi}{\sqrt{m D}} \quad (d = 1),
\]
\[
T_D = \frac{4\pi}{\sqrt{m D}} \quad (d = 2),
\]
\[
T_D = \frac{(6\pi^2)^{1/3}}{\sqrt{m D}} \quad (d = 3).
\] (132)

Replacing the integration according to the rule
\[
\int_B \frac{dk}{(2\pi)^d} \rightarrow \frac{d}{(k_D a)^d} \int_0^{k_D} k^{d-1} dk
\]
results in the mean square deviation
\[
r_0^2 = \frac{d}{2mT_D} \int_0^1 x^{d-2} \coth \left( \frac{T_D}{2T} x \right) dx.
\] (133)

At zero temperature, this yields
\[
r_0^2 = \frac{d^2}{2(d-1)mT_D} \quad (T = 0).
\] (134)

while at high temperature, we get
\[
r_0^2 \approx \frac{T_D^2}{(d-2)mT_D^2} \quad (T \gg T_D).
\] (135)

9. Stability of localized states

The stability of a localized state can be characterized by the Lindemann criterion [27], according to which the mean square deviation has to be smaller than half of the distance between the nearest neighbours,
\[
\frac{r_0}{a} < \frac{1}{2}.
\] (136)

otherwise strong atomic oscillations destroy the localization. With the mean square deviation (133), this criterion reads as
\[
\frac{12E_R}{\pi^2T_D} \int_0^1 x^{d-2} \coth \left( \frac{T_D}{2T} x \right) dx < 1,
\] (137)
where the recoil energy
\[
E_R = \frac{k_0^2}{2m} = \frac{\pi^2 d}{2ma^2}.
\] (138)

is introduced.

At zero temperature, the stability condition takes the form
\[
\frac{T_D}{E_R} > \frac{4d}{\pi^2(d-1)} \quad (T = 0).
\] (139)

Hence, one-dimensional periodic localized structures are not stable at zero temperature. While for higher dimensionalities, the stability condition gives
\[
\frac{T_D}{E_R} > \frac{8}{\pi^2} \quad (d = 2, \; T = 0).
\] (140)
\[
\frac{T_D}{E_R} > \frac{6}{\pi^2} \quad (d = 3, \; T = 0).
\] (141)

For temperatures above \(T_D\), the stability condition is
\[
\frac{T_D}{E_R} > \frac{8d}{\pi^2(d-2)} \quad (T \gg T_D).
\] (142)

At these temperatures, two-dimensional localized lattices are not stable. And the stability condition for a three-dimensional localized lattice is
\[
\frac{T_D}{E_R} > 2\frac{4}{\pi^2} \quad (d = 3, \; T \gg T_D).
\] (143)

It is possible to notice that the Debye temperature is very close to the frequency \(\Omega_\nu\) in definition (53). Really, their ratio is
\[
\frac{T_D}{\Omega_\nu} = \nu \sqrt{\frac{\pi}{d}} \left[ \frac{d}{2} \Gamma \left( \frac{d}{2} \right) \right]^{1/d}.
\] (143)

Taking for an estimate \(d = 3\), the number of the nearest neighbors \(2d = 6\), and the filling factor \(\nu = 1\), we get \(T_D = 1.1\Omega_\nu\).

In this way, the localized state is stable, when the interactions between different lattice sites are sufficiently strong,
such that the Debye temperature $T_D$ is essentially larger than the recoil energy $E_R$, with the above localization conditions being valid. When the latter do not hold, the system is not localized.

10. Classification of states

The character of a state realized in the system depends on the space dimensionality and the interplay between three types of the parameters, the optical-lattice frequencies that can be represented as

$$\omega_\alpha = \sqrt{\frac{4}{3} \frac{E_R U_\alpha}{\alpha}}, \quad (144)$$

the recoil energy $E_R$ and the Debye temperature $T_D$. The effective frequency of atomic oscillations (54) is regulated by both the optical-lattice frequency $\omega_\alpha$ and the Debye temperature $T_D$. As is clear from expressions (55) to (58), the atomic frequency $\omega_\alpha$ varies from $\omega_\alpha$ at weak intersite interactions to the Debye temperature $T_D$ under strong interactions between different lattice sites.

The behaviour of optical lattices, where there are no intersite interactions, hence $T_D = 0$, is well known, as can be inferred from the reviews [1–3] and books [4, 5]. At zero temperature, integer filling factor, and deep lattice, where $U_\alpha \gg E_R$, one has the Mott insulator, while in the opposite case of a shallow lattice, when $U_\alpha \ll E_R$, the optical lattice is conducting. If either temperatures are finite or the filling factor is not integer, the lattice cannot be completely localized, but is conducting. The inclusion of the intersite interactions makes the overall picture much more diversified. Summarizing the available knowledge on optical lattices without intersite interactions [1–3] and the results obtained in the previous sections, we have the following picture, where we keep in mind a three-dimensional system ($d = 3$).

Consider first the case of a deep optical lattice, such that

$$\frac{\omega_\alpha}{E_R} \gg 1 \quad \left(\frac{U_\alpha}{E_R} \gg 1\right). \quad (145)$$

If there are intersite interactions, so that $T_D > 0$, but they are rather weak,

$$0 \ll T_D \ll E_R \quad \left(\text{conducting optical lattice}\right), \quad (146)$$

we have a conducting optical lattice, with the lattice vector created by the applied laser beams. For intersite interactions much stronger than $E_R$, but smaller than $\omega_\alpha$, the optical lattice becomes insulating,

$$E_R \ll T_D \ll \omega_\alpha \quad \left(\text{insulating optical lattice}\right). \quad (147)$$

For even stronger intersite interactions, the insulating optical lattice transforms into a localized quantum crystal, with the lattice vector prescribed by the minimum of free energy,

$$E_R \ll \omega_\alpha \ll T_D \quad \left(\text{localized quantum crystal}\right). \quad (148)$$

If the imposed optical lattice is shallow, with $U_\alpha \ll E_R$, when

$$\frac{\omega_\alpha}{E_R} \ll 1 \quad \left(\frac{U_\alpha}{E_R} \ll 1\right), \quad (149)$$

then, depending on the strength of the intersite interactions, there can occur the following states. Under quite weak intersite interactions, when

$$0 \ll T_D \ll \omega_\alpha \quad \left(\text{conducting optical lattice}\right), \quad (150)$$

we have a conducting optical lattice. When the intersite interactions become prevailing over the optical-lattice potential, the system properties are governed by these interactions, but they may yet be not sufficient for localizing atoms, so that when

$$\omega_\alpha \ll T_D \ll E_R \quad \left(\text{delocalized quantum crystal}\right), \quad (151)$$

there happens a delocalized quantum crystal. And when the intersite interactions are larger than all other potentials,

$$\omega_\alpha \ll E_R \ll T_D \quad \left(\text{localized quantum crystal}\right), \quad (152)$$

the quantum crystal localizes. Recall that this classification concerns three-dimensional systems.

11. Low-dimensional finite localized lattices

As is shown in section 9, one-dimensional localized lattices cannot exist at any temperature, including zero temperature, and two-dimensional localized lattices cannot exist at finite temperatures. These conclusions have been obtained for macroscopic periodic systems, for which the minimal wave-vector in the Brillouin zone is zero. But if the system is finite, the minimal wave-vector is limited because of the finite-size effects, being of the order of

$$k_{\min} = \frac{\pi}{L} \quad \left(L = N_L^{1/d} a\right). \quad (153)$$

Then the integral in equation (133) is limited from below by the quantity

$$x_{\min} \equiv \frac{k_{\min}}{k_D} = -\frac{\pi}{k_D a N_L^{1/d}} \quad (154)$$

that is asymptotically small with respect to $N_L$, but finite,

$$x_{\min} = \frac{1}{N_L} \quad (d = 1), \quad (155)$$

$$x_{\min} = \frac{1}{2} \sqrt{\frac{\pi}{N_L}} \quad (d = 2). \quad (156)$$

For a one-dimensional system at zero temperature, equation (133) gives

$$r_0^1 \approx \frac{\ln N_L}{2m T_D} \quad (d = 1, \ T = 0), \quad (157)$$

while for a two-dimensional system $r_0^2 = 2/m T_D$. This means that two-dimensional localized lattices can be of any size, while the size of one-dimensional localized lattices is restricted by the inequality

$$N_L < \exp\left(\frac{\pi^2 T_D}{4E_R}\right) \quad (d = 1, \ T = 0). \quad (158)$$
following from the Lindemann stability condition \((136)\).

At finite temperature, equation \((133)\) results in the expressions

\[
r_0^2 \cong \frac{TN_l}{mT_D} \quad (d = 1, \ T > 0)
\]

\[
r_0^2 \cong \frac{T \ln N_l}{mT_D} \quad (d = 2, \ T > 0).
\]

Therefore, the Lindemann criterion imposes the constraints

\[
N_L < \frac{\pi^2 T_D^3}{8TE_R} \quad (d = 1, \ T > 0),
\]

\[
N_L < \exp \left( \frac{\pi^2 T_D^2}{4TE_R} \right) \quad (d = 2, \ T > 0) \quad (158)
\]

on the size of localized lattices. Such a size, depending on the parameters, can be quite large. Take, for instance, \(T \sim T_D \sim 10E_R\). Then finite localized lattices can contain the number of lattice sites as \(N_L < 10^4\) for \(d = 1\) and \(N_L < 5 \times 10^{10}\) for \(d = 2\).

Thus one- and two-dimensional localized structures can exist as finite objects, with the sizes prescribed by temperature, recoil energy, and the strength of intersite interactions characterized by the Debye temperature. Such finite localized structures can exist even if the corresponding macroscopic objects are not localized.

12. Conclusion

In this paper, we consider optical lattices of atoms or molecules that, in addition to one-site interactions, exhibit interactions between different lattice sites. These intersite interactions can be rather strong, inducing collective phonon excitations above the ground-state energy level. The properties of optical lattices in the case of absent intersite interactions are known. We pose the question: What happens if the strength of the intersite interactions increases, from the situation where this strength is much weaker than the optical lattice potential and the system properties are governed by the optical lattice to the case where the strength of the intersite interactions is much larger than the optical potential barrier? The properties of the system are shown to be mainly regulated by the three types of the system parameters, optical-lattice frequencies, recoil energy, and the Debye temperature characterizing the strength of the intersite atomic interactions. Depending on the interplay between these parameters, in three dimensions, there can exist conducting optical lattices, insulating optical lattices, delocalized quantum crystals, and localized quantum crystals.

In one-dimensional systems, localized macroscopic lattice structures cannot arise at any temperature, either zero or not. And in two dimensions, localized lattices can arise only at zero temperature. Nevertheless, one-dimensional localized chains and two-dimensional plains of localized atoms can exist at zero as well as at nonzero temperature, provided such low-dimensional structures are of finite sizes.

The consideration in the paper concerns equilibrium systems. It is also possible to mention that even if an equilibrium system cannot occur, there can be created a similar metastable system with sufficiently long lifetime. Thus, assume that an insulating lattice is unstable as an equilibrium system. Anyway, it can be created as a metastable object with the lifetime

\[
t_{\text{met}} = \min \frac{2\pi}{\omega_\alpha} \exp \left( \frac{U_\alpha}{E_R} \right).
\]

The existence of long-lived metastable systems, as well as the occurrence of stable finite low-dimensional localized lattices of chains and planes, explains why such structures can be created and studied in experiments. In the present paper, we have considered the destiny of optical lattices, loaded by atoms or molecules with strong intersite interactions inducing collective excitations. Similar investigations could be appropriate for other finite quantum systems, whose stability, and hence existence, are intimately connected with the presence of collective excitations \([28]\).

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