From optical lattices to quantum crystals

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Abstract. Optical lattices can be loaded with atoms which can have strong interactions, such that the interaction of atoms at different lattice sites cannot be neglected. Moreover, the intersite interactions can be so strong that it can force the atoms to form a self-organized lattice, such that exists in crystals. With increasing intersite interactions, there can appear several lattice states, including conducting optical lattices, insulating optical lattices, delocalized quantum crystals, and localized quantum crystals.

1. Introduction

Optical lattices can be created by laser beams and loaded with different atoms and molecules [1]. The standard situation is when atoms, or molecules, interact with each other through local forces modelled by the delta-function potential [2–5]. With such a short-range potential, the interactions of atoms at different lattice sites are negligible, and only onsite interactions are taken into account. There exist also long-range potentials, such as dipolar, for which it is necessary to take account of intersite interactions [6–13]. Usually dipolar potentials are treated as weak, in comparison to local potentials. However, if they are sufficiently strong, they can lead to roton instability inducing self-organized droplet crystals, which also appear for atoms with some soft-core repulsive interactions [14].

Actually, it is well known that atoms with sufficiently strong interactions, not necessarily of long-range type, can form self-organized periodic structures, that is crystals. When quantum properties are important, one has quantum crystals [15–17]. Thus it looks to be clear that under weak atomic (molecular) interactions, but in the presence of external periodic fields forming a lattice, there is the usual optical lattice, with the lattice parameters prescribed by external laser fields. While when intersite interactions are sufficiently strong, a self-organized periodic structure can develop. Our aim is to understand what happens between these two limiting states, an optical lattice and a quantum crystal.

It is also well known that optical lattices can house either nonlocalized or localized atoms. If the atoms in the lattice are not localized, they can be in a normal state or in a superfluid state. Nonlocalized states are often termed conducting. But our aim is not to study phase transitions between normal and superfluid nonlocalized states, but to distinguish between localized and nonlocalized (conducting) states.

Keeping in mind to find a stability boundary between two phases, without investigating the details of the related phase transition itself, it is not compulsory to study both the neighbouring
phases at both sides of this boundary. But it is sufficient to study the system stability from one side of the boundary. This is what is done in the present paper by determining the stability boundary from the side of a localized state. The main aim is to find out what states, from the point of view of particle localization, can arise under the variation of atomic interactions from weak, when the system presents a simple optical lattice, to strong, when the lattice structure is caused by atomic interactions. That is, the aim is to classify possible states arising, under the strengthening of atomic interactions, between the standard optical lattices and quantum crystals.

The system of units is employed, where the Planck and Boltzmann constants are set to one.

2. Localized states

A system of atoms, with mass \( m \), interacting by means of a pair potential \( \Phi(r) \), is also subject to laser beams creating an optical lattice with a periodic potential

\[
U_L \left( r + \frac{\lambda_\alpha}{2} \right) = U_L(r),
\]

with the lattice spacing \( \lambda_\alpha/2 \) in the direction labeled by \( \alpha = 1, 2, \ldots, d \), where \( d \) is the space dimensionality. The typical lattice potential is

\[
U_L(r) = \sum_{\alpha=1}^{d} U_\alpha \sin^2(k_\alpha^0 r_\alpha),
\]

where \( k_\alpha^0 = \frac{2\pi}{\lambda_\alpha} \).

The system Hamiltonian is

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

where

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

is the lattice Hamiltonian.

Field operators obey either Bose or Fermi statistics, which for a well localized state is of no importance. Keeping in mind a localized state, the field operators can be expanded over well localized Wannier functions \[18\]

\[
\psi^\dagger(r) = \sum_{j=1}^{N_L} \hat{c}_j w(r - r_j),
\]

where the single-band approximation is assumed and \( N_L \) is the number of sites.

Substituting expansion (5) into the Hamiltonian gives the form \[19\]

\[
\hat{H} = -\sum_{i \neq j} J_{ij} \hat{c}_i^\dagger \hat{c}_j + \sum_j \left( \frac{p_j^2}{2m} + U_L \right) \hat{c}_j^\dagger \hat{c}_j + \frac{1}{2} \sum_j U_{jj} \hat{c}_j^\dagger \hat{c}_j^\dagger \hat{c}_j \hat{c}_j + \frac{1}{2} \sum_{i \neq j} U_{ij} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_j \hat{c}_i,
\]

in which the notation is used for the tunneling matrix

\[
J_{ij} = -\int w^*(r - r_i) \hat{H}_L(r) w(r - r_j) \, dr \quad (i \neq j),
\]
the matrix element for the momentum squared
\[ P_j^2 = \int w^*(r - r_j)(-\nabla^2)w(r - r_j) \, dr , \tag{8} \]
the lattice Hamiltonian parameter
\[ U_L = \int |w(r)|^2 U_L(r) \, dr , \tag{9} \]
and the interaction matrix
\[ U_{ij} = \int |w(r - r_i)|^2 \Phi(r - r_j)|w(r' - r_j)|^2 \, dr \, dr'. \tag{10} \]

The density of atoms is
\[ \rho(r) = \langle \hat{\psi}^\dagger(r)\hat{\psi}(r) \rangle = \sum_{ij} \langle \hat{c}_i^\dagger \hat{c}_j \rangle |w^*(r - r_i)w(r - r_j)|^2 . \tag{11} \]

We keep in mind a well localized lattice, assuming the use of well localized Wannier functions [18]. Under the assumption of strong localization, the intersite tunneling of atoms can be neglected setting
\[ \hat{c}_i^\dagger \hat{c}_j = \nu \delta_{ij} \left( \nu \equiv \frac{N}{N_L} \right) , \tag{12} \]

with \( \nu \) filling factor. Then the density of atoms (11) reads
\[ \rho(r) = \nu \sum_j |w(r - r_j)|^2 . \tag{13} \]

3. Energy of atoms
Atomic energy levels can be defined [20,21] as the eigenvalues of the eigenproblem
\[ \int H(r, r', \omega)\varphi_{nk}(r') \, dr' = E_{nk}\varphi_{nk}(r) \tag{14} \]
for the effective Hamiltonian
\[ H(r, r', \omega) = -\frac{\nabla^2}{2m} \delta(r - r') + \Sigma(r, r', \omega) , \tag{15} \]

in which \( \Sigma \) is self-energy. For well localized particles, the self-energy can be taken [15–17] in the Hartree approximation
\[ \Sigma(r, r', \omega) = [ U_L(r) + V_H(r) ]\delta(r - r') , \tag{16} \]

with the Hartree potential
\[ V_H(r) = \int \Phi(r - r')\rho(r') \, dr' . \tag{17} \]

Then eigenproblem (14) reduces to the equation
\[ \hat{H}(\varphi_{nk}(r) = E_{nk}\varphi_{nk}(r) , \tag{18} \]

with the periodic Hamiltonian
\[ \hat{H}(r) = \hat{H}_L(r) + V_H(r) = \hat{H}(r + r_j) , \tag{19} \]
whose eigenfunctions are, clearly, Bloch functions.

It is useful to mention that, generally, Wannier functions are not the eigenfunctions of Hamiltonian (19). To see this, it is sufficient to expand the Bloch function over Wannier functions,

$$\varphi_{nk}(r) = \frac{1}{\sqrt{NL}} \sum_j w_n(r - r_j)e^{i\mathbf{k} \cdot \mathbf{r}_j},$$

which transforms eigenproblem (18) into the equation

$$\hat{H}(r)w_n(r - r_j) = \sum_i E^n_{ij} w_n(r - r_i),$$

in which

$$E^n_{ij} \equiv \frac{1}{NL} \sum_k E_{nk}e^{i\mathbf{k} \cdot \mathbf{r}_{ij}} \quad (\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j).$$

The eigenfunctions of Hamiltonian (19) are not separate Wannier functions but the lattice sums

$$\psi_n(r) = \sum_j w_n(r - r_j)$$

that are the eigenfunctions satisfying the eigenproblem

$$\hat{H}(r)\psi_n(r) = E_n\psi_n(r),$$

with the eigenvalues

$$E_n \equiv \sum_j E^n_{ij} = \lim_{k \to 0} E_{nk}.$$

For well localized Wannier functions, we have

$$\psi_n(r) \approx w_n(r - r_j) \quad (r \approx r_j).$$

In that case, Wannier functions play the role of approximate eigenfunctions of Hamiltonian (19). For the lowest band, we get

$$\hat{H}(r)w(r) = Ew(r) \quad (r \approx 0).$$

The solution to equation (26) can be found by means of optimized perturbation theory [22]. For the initial approximation, it is natural to take a harmonic Hamiltonian

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

with the potential

$$U_0(r) = u_0 + \sum_\alpha m \frac{\epsilon_\alpha^2 r_\alpha^2}{2},$$

which yields the Gaussian wave function

$$w(r) = \prod_\alpha \left( \frac{1}{\pi l_\alpha^2} \right)^{1/4} \exp \left( -\frac{r_\alpha^2}{2l_\alpha^2} \right),$$

where $l_\alpha \equiv 1/\sqrt{m \epsilon_\alpha}$. The frequency $\epsilon_\alpha$ is the control parameter to be found from optimization conditions [22].
The energy, corresponding to Hamiltonian (27), reads
\[ E_0 = u_0 + \frac{1}{2} \sum_\alpha \varepsilon_\alpha. \]  
(30)

And to first order of perturbation theory, the eigenvalue of equation (26) is
\[ E_1 = \int w(r) \hat{H}_1(r) w(r) \, dr, \]  
(31)

where
\[ \hat{H}_1(r) = -\frac{\nabla^2}{2m} + U_1(r), \quad U_1(r) = U_L(r) + V_1(r), \]
\[ V_1(r) = \int \Phi(r-r') \rho_0(r') \, dr', \quad \rho_0(r) = \nu \sum_j w^2(r-r_j). \]

As an optimization condition, it is convenient to take the equality
\[ E_1 - E_0 = 0. \]  
(32)

For small \( r \), the lattice potential (2) can be written as
\[ U_L(r) \simeq \sum_\alpha \frac{m}{2} \omega_\alpha^2 r^2_\alpha \quad (r \approx 0), \]  
(33)

with the frequency
\[ \omega_\alpha = 2 \sqrt{E_R^\alpha U_\alpha} \quad \left( E_R^\alpha \equiv \frac{(k_0^\alpha)^2}{2m} \right). \]  
(34)

Then for energy (31) it follows
\[ E_1 = u_0 + \frac{1}{4} \sum_\alpha \left( \varepsilon_\alpha + \frac{\omega_\alpha^2}{\varepsilon_\alpha} + \frac{\Omega_\alpha^2}{\varepsilon_\alpha} \right), \]  
(35)

where
\[ \Omega_\alpha \equiv \left[ \frac{2\nu}{m} \sum_j \frac{\partial^2 \Phi(r_j)}{\partial r_j^\alpha \partial r_j^\alpha} \right]^{1/2}. \]  
(36)

Setting
\[ u_0 = \nu \sum_j \Phi(r_j), \]  
(37)

we find the effective frequency of atomic oscillations
\[ \varepsilon_\alpha = \sqrt{\omega_\alpha^2 + \Omega_\alpha^2}. \]  
(38)

As is seen, the effective frequency of atomic oscillations is formed both, by the lattice potential and by direct atomic interactions. When the atomic interaction potential grows from zero to a strong \( \Phi(r) \), the effective frequency increases from \( \omega_\alpha \), created by the optical lattice, to \( \Omega_\alpha \), due to atomic interactions. Let us mention that in the case of well localized atoms, the intersite tunneling is suppressed, which is evident from the expression for the tunneling parameter
\[ J_{ij} = \sum_\alpha \left\{ \frac{\varepsilon_\alpha}{8} \left[ \left( \frac{r_{ij}^\alpha}{l_\alpha} \right)^2 - 2 \right] - U_\alpha \right\} \exp \left\{ -\frac{1}{4} \sum_\alpha \left( \frac{r_{ij}^\alpha}{l_\alpha} \right)^2 \right\}. \]
4. Phonon excitations

The lowest atomic band corresponds to the ground-state energy. Above this energy there exist collective atomic excitations represented by phonon degrees of freedom. Phonon variables can be introduced as it has been done, e.g., in Refs. [23–25]. The vector $\mathbf{r}$ is treated as an operator written in the form

$$ r_j = a_j + u_j , $$

(39)

in which $a_j$ is an equilibrium position defining an effective lattice site, while $u_j$ is a deviation from the site. Thus the averages

$$ a_j = \langle r_j \rangle, \quad \langle u_j \rangle = 0, $$

(40)

are assumed to be valid by definition.

Note that the actual positions of the effective lattice sites $a_j$ are given by the minimization of a thermodynamic potential. This implies that the parameters of the effective lattice are defined by the joint action of the imposed optical lattice and by atomic interactions.

An important quantity is the mean-square atomic deviation

$$ r_0^2 = \sum_{\alpha=1}^{d} \langle u_\alpha^2 u_\alpha^2 \rangle. $$

(41)

In the Debye approximation, we find [24, 25]

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

(42)

where the integration is over the Brillouin zone and the phonon frequency is defined by the expression

$$ \omega_k^2 = \frac{4\nu}{m} D \sum_{\alpha=1}^{d} \sin^2 \left( \frac{k_\alpha a}{2} \right), $$

(43)

with the notation for the dynamic parameter

$$ D = \frac{\nu^2}{d} \sum_{\alpha} \frac{\partial^2 U(a)}{\partial a^\alpha \partial a^\alpha}, $$

(44)

in which

$$ U(a_{ij}) = \int | w(\mathbf{r} - a_i) |^2 \Phi(\mathbf{r} - \mathbf{r}') | w(\mathbf{r}' - a_j) |^2 d\mathbf{r} d\mathbf{r}' $$

and where the nearest-neighbour approximation is used, with $a$ being the nearest-neighbour distance.

The long-wave limit gives the phonon spectrum

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

(45)

with the sound velocity

$$ c_0 = \sqrt{\frac{\nu}{m} Da^2}. $$

(46)
In the Debye approximation, the phonon spectrum is limited by the Debye wave vector

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

The phonon excitations do not destroy localized states, provided the Lindemann criterion of stability holds true \[26\]. According to this criterion, a localized state can be stable, if the mean-square deviation is smaller than half of the nearest-neighbour distance,

\[ \frac{r_0}{a} < \frac{1}{2}. \] (47)

Otherwise, the localized state is not stable. In the Debye approximation, the stability criterion reads

\[ 12 \frac{E_K}{T_D} \int_0^1 x^{d-2} \coth \left( \frac{T_D}{2T} x \right) dx < 1, \] (48)

where the Debye temperature is

\[ T_D = \sqrt{\frac{4\pi \nu D}{m}} \left[ \frac{d}{2} \Gamma \left( \frac{d}{2} \right) \right]^{1/d} \] (49)

and \( E_K \) is a characteristic kinetic energy

\[ E_K \equiv \frac{1}{2ma^2}. \] (50)

At zero temperature, the localized state is stable under the condition

\[ \frac{T_D}{E_K} > \frac{4d^2}{d-1} \quad (T = 0). \] (51)

This means that a one-dimensional crystal is not stable. The criterion for a two-dimensional crystal is

\[ \frac{T_D}{E_K} > 16 \quad (d = 2, \ T = 0). \] (52)

And a three-dimensional crystal at zero temperature can be stable, if

\[ \frac{T_D}{E_K} > 18 \quad (d = 3, \ T = 0). \] (53)

At high temperatures, the criterion becomes

\[ \frac{T_D}{E_K} > \frac{8d^2}{d-2} \quad (T \gg T_D). \] (54)

Hence only a three-dimensional crystal can be stable, provided that

\[ \frac{T_D}{E_K} > 72 \quad (d = 3, \ T \gg T_D). \] (55)

For a three-dimensional system, the oscillation frequency (36), caused by atomic interactions, is close to the Debye temperature (49) and the recoil energy \( E_R \) is close to the characteristic kinetic energy \( E_K \). The system state depends of the relation between three main parameters, the
frequency $\omega_\alpha$, defined by the optical lattice, the characteristic kinetic energy $E_K$, and the Debye temperature $T_D$. Summarizing the available information and assuming that the frequencies $\omega_\alpha$ are close to each other, we find the following classification of possible states.

If the imposed optical lattice is shallow, such that $\omega_\alpha \ll E_K$, then, depending on the relation between the other parameters, there can exist the following states. If $0 \leq T_D \ll \omega_\alpha$, the system forms a conducting optical lattice. When $\omega_\alpha \ll T_D \ll E_K$, a delocalized quantum crystal can arise. For $\omega_\alpha \ll E_K \ll T_D$, a localized quantum crystal is stable.

When the optical lattice is sufficiently deep, so that $\omega_\alpha \gg E_K$, then the following states are possible. Here we keep in mind the general situation with an arbitrary filling factor and temperature. The case of an integer filling factor and zero temperature is special, requiring to take account of the onsite interactions [2–5]. If $0 < T_D \ll \omega_\alpha$, we have a conducting optical lattice. When $E_K \ll T_D \ll \omega_\alpha$, the optical lattice becomes insulating. And for $E_K \ll \omega_\alpha \ll T_D$, a localized quantum crystal is formed.

Concluding, the role of intersite interactions is investigated for a system of atoms in an optical lattice. In the absence of the intersite interactions, all properties of the system are governed by the optical lattice. But in the presence of the intersite interactions, collective phonon excitations can arise, and the system state can be strongly changed. This state is mainly regulated by the relations between three parameters, the frequency $\omega_\alpha$, caused by the optical lattice, the characteristic kinetic energy $E_K$, that is close to the recoil energy, and the Debye temperature $T_D$, whose existence and strength are due to the intersite interactions. A three-dimensional system, with an arbitrary filling factor and temperature, can be in four different states forming either a conducting optical lattice, or an insulating optical lattice, or a delocalized quantum crystal, or a localized quantum crystal. In a quantum crystal there also exists a lattice. But the difference between an optical lattice and a crystalline lattice is in their origins. An optical lattice is created by external laser beams prescribing the lattice period and depth. In contrast, a crystalline lattice is formed self-consistently, due to atomic interactions, providing a state realizing a minimum of thermodynamic potential.

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