Cold atoms in double-well optical lattices

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Abstract

Cold atoms, loaded into an optical lattice with double-well sites, are considered. Pseudospin representation for an effective Hamiltonian is derived. The system in equilibrium displays two phases, ordered and disordered. The second-order phase transition between the phases can be driven either by temperature or by changing the system parameters. Collective pseudospin excitations have a gap disappearing at the phase-transition point. Dynamics of atoms is studied, when they are loaded into the lattice in an initially nonequilibrium state. It is shown that the temporal evolution of atoms, contrary to their equilibrium thermodynamics, cannot be described in the mean-field approximation, since it results in a structurally unstable dynamical system, but a more accurate description is necessary taking account of attenuation effects.

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I Introduction

Degenerate cold gases, Bose [1–8] as well as Fermi [9,10], possess many interesting properties. Loading cold atoms into optical lattices yields highly controllable systems that could be employed for a variety of applications [11–15]. Recently, a novel type of optical lattices has been experimentally realized, each site of which is formed by a double-well potential [16–21].

The phase diagram of cold bosons in double-well optical lattices has been studied in Refs. [22,23], where the Hubbard model is used and the main attention is payed to the peculiarities of the superfluid-insulator phase transition in such lattices, as compared to this transition in the standard single-well optical lattices [11–14]. In Ref. [24], the superfluid phase is studied, aiming at finding a type of superfluid with the broken time-reversal symmetry.

The aim of the present paper is to study a different regime that can be realized in the double-well optical lattices. We consider the lattices that are in the insulating state, far from the boundary of the insulator-superfluid transition. In that state, the jumps of atoms between different lattice sites are suppressed, while the tunneling between the wells of a single-site double well can be of principal importance. We show that in such insulating double-well optical lattices there exists another phase transition, the order-disorder phase transition. The investigation of this different physical regime in insulating double-well optical lattices, far from the superfluid phase-transition, but close to another, order-disorder phase transition, is the main motivation for the present work.

The order-disorder phase transition, and the related ordered and disordered states, can be the most clearly realized for the case of one atom per a double well. Therefore, we consider exactly this case. An additional argument for considering the lattices with one atom per site is that the optical lattices with small filling factors, such as one or two, seem to be good candidates for quantum information processing [11,19].

The advantage of dealing with the case of one atom per a double well is twofold. The most important, as is emphasized above, is that this is the setup allowing for a clear realization of the order-disorder phase transition. Another, technical, convenience is that in this case the pseudospin representation can be invoked. Some types of spin Hamiltonians using cold atoms in optical lattices can be met in literature. It is straightforward to obtain a spin Hamiltonian for spinor condensates [25]. The Hubbard model for a system of two-component bosons can be reduced to a pseudospin representation by a second-order perturbation theory in the tunneling parameter [26–28]. In our case of an insulating double-well optical lattice, the pseudospin representation can be introduced without perturbation theory, by means of an exact canonical transformation, similar to the canonical transformations used for deriving the spin representations for superconductors and ferromagnets [29,30].

The key point of realizing the ordered and disordered states in a double-well optical lattice is the existence of sufficiently long-range atomic interactions. Such interactions of dipolar type arise between polar molecules [31], Rydberg atoms [32], and between atoms with large magnetic moments [33]. The existence of long-range atomic interactions is another point making our consideration principally different from the earlier theoretical works [22–24] on the double-well lattices.
Characterizing collective atomic states in the double-well lattices, we, first, describe their equilibrium properties. However, we keep in mind that in experiments atoms need to be loaded into a lattice, and their initial state after the loading may be nonequilibrium. If so, how then atoms would relax to their equilibrium state? Another way, when atoms can happen to be in a nonequilibrium states, is if the lattice parameters are varied after the atoms have been loaded. If this variation is sufficiently fast, atoms again occur to be in a nonequilibrium state, from which they should relax to an equilibrium one. In order that our consideration of the insulating double-well optical lattices would be more complete, and keeping in mind the possibility of realizing nonequilibrium states, we study not only the equilibrium properties of such lattices, but also the relaxational dynamics of atoms from initially nonequilibrium states to their equilibrium.

The paper is organized as follows. First, we derive an effective Hamiltonian for the considered insulating system and show that it allows for a convenient pseudospin representation (Sec. II). Then we study the equilibrium thermodynamics of the model, which exhibits the existence of two phases, ordered and disordered (Sec. III). Collective excitations, corresponding to pseudospin waves, are described in Sec. IV. Dynamics of atoms, loaded in the lattice in an initially nonequilibrium state, is considered in Sec. V. Lyapunov stability and structural stability of solutions to the equations of motion are investigated in Sec. VI, where the principal importance of taking into account attenuation effects is demonstrated. The main results are summarized in Sec. VII.

**II Model Hamiltonian**

We start with the general form of the energy Hamiltonian

\[ \hat{H} = \int \psi^\dagger(\mathbf{r}) H_L(\mathbf{r}) \psi(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \int \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}) \, d\mathbf{r} d\mathbf{r}' , \]  

where \( \psi(\mathbf{r}) = \psi(\mathbf{r}, t) \) is a field operator, in which the time dependence, for brevity, is omitted. Keeping in mind the case of an insulating lattice, with the unity filling factor, the statistics of atoms is not as important. So, atoms can be either bosons or fermions. In the lattice Hamiltonian

\[ H_L(\mathbf{r}) \equiv - \frac{\nabla^2}{2m} + V(\mathbf{r}) , \]  

the lattice potential \( V(\mathbf{r} + \mathbf{a}_i) = V(\mathbf{r}) \) is periodic over the lattice \( \{ \mathbf{a}_i : i = 1, 2, \ldots, N_L \} \) and enjoys the double-well structure around each of the lattice sites \( \mathbf{a}_i \). The interaction potential \( \Phi(-\mathbf{r}) = \Phi(\mathbf{r}) \), in general, is a sum of the short-range interactions, whose strength can be regulated by the Feschbach resonance techniques [2,10,15,34,35], and of a long-range interaction of the dipolar type, such that exists between polar molecules [31], Rydberg atoms [32], and atoms with large magnetic moments [33]. If, instead of atoms, we consider ions, then these exists the long-range Coulomb interaction. The strength of the interaction potential is assumed to be such that the intersite interactions, at least between the nearest neighbors, cannot be neglected.

The field operator can be expanded over Wannier functions

\[ \psi(\mathbf{r}) = \sum_{nj} c_{nj} w_n(\mathbf{r} - \mathbf{a}_j) , \]  

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where \( n \) is a band index and \( j \) enumerates the lattice sites. Then Hamiltonian (1) transforms into

\[
\hat{H} = \sum_{ij} \sum_{mn} E_{ij}^{mn} c_{mi}^\dagger c_{nj} + \frac{1}{2} \sum_{\{j\}} \sum_{\{n\}} \Phi_{j1j2j3j4}^{n1n2n3n4} c_{n1j1}^\dagger c_{n2j2}^\dagger c_{n3j3} c_{n4j4} ,
\]

where

\[
E_{ij}^{mn} \equiv \int w_m^*(\mathbf{r} - \mathbf{a}_i) H_L(\mathbf{r}) w_n(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r}
\]

and \( \Phi_{j1j2j3j4}^{n1n2n3n4} \) is the corresponding matrix element of the interaction potential.

It can be shown (see Appendix A), that

\[
E_{ij}^{mn} = \delta_{mn} E_{ij}^n
\]

is diagonal with respect to the band indices. Here,

\[
E_{ij}^n = \delta_{ij} E_n + (1 - \delta_{ij}) J_{ij}^n
\]

with

\[
E_n = \int w_n^*(\mathbf{r}) H_L(\mathbf{r}) w_n(\mathbf{r}) \, d\mathbf{r} , \quad J_{ij}^n = \int w_n^*(\mathbf{r} - \mathbf{a}_{ij}) H_L(\mathbf{r}) w_n(\mathbf{r}) \, d\mathbf{r} .
\]

Keeping in mind an insulating lattice implies that the intersite hopping is small, such that

\[
\left| \frac{J_{ij}}{E_n} \right| \ll 1 \quad (i \neq j) .
\]

Assuming that each lattice site contains just one atom, we impose the unipolarity conditions

\[
\sum_n c_{nj}^\dagger c_{nj} = 1 , \quad c_{nj} c_{nj} = 0 .
\]

Taking into account the above consideration, for Hamiltonian (4) we have

\[
\hat{H} = \sum_{nj} E_n c_{nj}^\dagger c_{nj} + \frac{1}{2} \sum_{i \neq j} \sum_{mnm'_{n'}} V_{ij}^{nmn'_{n'}} c_{mi}^\dagger c_{nj}^\dagger c_{m'_{n'}j} c_{n'i} ,
\]

where

\[
V_{ij}^{nmn'_{n'}} \equiv \Phi_{ijij}^{nmn'_{n'}} \pm \Phi_{ijij}^{nmn'_{n'}} ,
\]

with the upper or lower sign for bosons or fermions, respectively.

When a single-well potential is transformed into a double-well potential, then each spectrum level of a particle, it would possess in the former potential, splits into two lines for the particle in a double-well potential. The spectrum splitting is connected with the particle tunneling between the wells of a double-well potential. The splitting magnitude depends on the characteristics of the double-well potential and can be regulated in a wide range [36]. Thus, for a double-well lattice, one cannot limit oneself by considering solely the lowest energy band, but at least two energy levels must be taken into account, describing the level splitting and interwell tunneling. In what follows, we take into account two lowest energy levels, so that the index \( n \) takes two values \( n = 1, 2 \).
The symmetry properties of the ground-state wave function and of that for the first excited state are known [36] to be different. Enumerating the ground state with \( n = 1 \) and the excited state with \( n = 2 \), one has

\[
w_1(-r) = w_1(r) , \quad w_2(-r) = -w_2(r) .
\]

(12)

Also, both functions \( w_n(r) \), for \( n = 1, 2 \), can be taken to be real. Because of the symmetry property (12), the matrix elements of the type as \( V_{ij}^{1112} \) and \( V_{ij}^{2221} \) become zero.

For what follows, it is convenient to introduce the notation

\[
E_0 \equiv \frac{1}{2} (E_1 + E_2) .
\]

(13)

And let us define the interaction matrix elements

\[
A_{ij} \equiv \frac{1}{4} \left( V_{ij}^{1111} + V_{ij}^{2222} + 2V_{ij}^{1221} \right) , \quad B_{ij} \equiv \frac{1}{2} \left( V_{ij}^{1111} + V_{ij}^{2222} - 2V_{ij}^{1221} \right) ,
\]

\[
C_{ij} \equiv \frac{1}{2} \left( V_{ij}^{2222} - V_{ij}^{1111} \right) , \quad I_{ij} \equiv -2V_{ij}^{1122} .
\]

(14)

The quantity

\[
\Omega \equiv E_2 - E_1 + \sum_{j(\neq i)} C_{ij}
\]

is the tunneling frequency characterizing the tunneling between the wells of a double-well potential.

The convenience of dealing with the two-level case is that it allows for the introduction of the pseudospin representation. The pseudospin operators can be defined as

\[
S_j^x = \frac{1}{2} \left( c_{j1}^\dagger c_{j1} - c_{j2}^\dagger c_{j2} \right) , \quad S_j^y = \frac{i}{2} \left( c_{j1}^\dagger c_{j2} - c_{j2}^\dagger c_{j1} \right) , \quad S_j^z = \frac{1}{2} \left( c_{j1}^\dagger c_{j2} + c_{j2}^\dagger c_{j1} \right) ,
\]

(16)

which gives

\[
c_{j1}^\dagger c_{j1} = \frac{1}{2} + S_j^x , \quad c_{j2}^\dagger c_{j2} = \frac{1}{2} - S_j^x , \quad c_{j1}^\dagger c_{j2} = S_j^x - iS_j^y , \quad c_{j2}^\dagger c_{j1} = S_j^x + iS_j^y .
\]

(17)

The physical meaning of the pseudospin operators (16) can be clarified by introducing the left, \( c_{jL} \), and the right, \( c_{jR} \), location operators

\[
c_{jL} \equiv \frac{1}{\sqrt{2}} \left( c_{j1} + c_{j2} \right) , \quad c_{jR} \equiv \frac{1}{\sqrt{2}} \left( c_{j1} - c_{j2} \right) ,
\]

(18)

characterizing the left or right location of an atom in the left or right well of a double-well potential. The pseudospin operators (16), expressed through the location operators (18), become

\[
S_j^x = \frac{1}{2} \left( c_{jL}^\dagger c_{jR} + c_{jR}^\dagger c_{jL} \right) , \quad S_j^y = -\frac{i}{2} \left( c_{jL}^\dagger c_{jR} - c_{jR}^\dagger c_{jL} \right) ,
\]

\[
S_j^z = \frac{1}{2} \left( c_{jL}^\dagger c_{jL} + c_{jR}^\dagger c_{jR} \right) .
\]
\[ S_j^z = \frac{1}{2} \left( c_j^\dagger c_j^L - c_{jR}^\dagger c_{jR} \right) . \]  

(19)

This representation demonstrates that \( S_j^x \) characterizes the tunneling intensity between the left and right wells of a double-well potential centered at the \( j \)-site; the operator \( S_j^y \) corresponds to the Josephson current between the wells; while \( S_j^z \) is the displacement operator describing imbalance between the wells.

Finally, for Hamiltonian (10), we obtain the pseudospin form

\[ \hat{H} = E_0 N + \frac{1}{2} \sum_{i \neq j} A_{ij} - \Omega \sum_j S_j^x + \sum_{i \neq j} B_{ij} S_i^x S_j^x - \sum_{i \neq j} I_{ij} S_i^z S_j^z . \]  

(20)

The first two terms here are not of the operator type, hence, can be omitted. The third term describes the tunneling between the wells of a double-well potential at the \( j \)-site, with the tunneling frequency \( \Omega \). The fourth and fifth terms characterize particle interactions, with the transverse strength \( B_{ij} \) and longitudinal strength \( I_{ij} \). The values of the system parameters depend on the properties of particle interactions and on the features of the lattice potential. Generally, these parameters can be varied in rather wide ranges.

In order to illustrate how the tunneling frequency (15) can be varied, we may take the double-well potential, in the vicinity of the lattice site \( a_j = 0 \), in the form

\[ V(r) \simeq V_0 \left( \frac{r_x}{r_0} \right)^2 \left[ \left( \frac{r_z}{r_0} \right)^2 - 2 \right] + V_H(r_y, r_z) , \]

where \( V_H(r_y, r_z) \) is a harmonic potential in the \( y \)- and \( z \)-directions. The tunneling frequency \( \Omega \) essentially depends on the parameters of the double-well potential \( V(r) \), its depth \( V_0 \) and the interwell distance \( r_0 \). These parameters enter the variable

\[ \alpha \equiv \frac{1}{\sqrt{2mr_0^2V_0}} , \]

which varies in the interval \( 0 < \alpha < \infty \). For intermediate values of \( \alpha \), the tunneling frequency can be calculated numerically, while for small and large \( \alpha \), asymptotic expressions are available [36] yielding

\[ \Omega \simeq 6V_0 \exp \left( \frac{2}{\alpha} \right) \quad (\alpha \ll 1) , \]

\[ \Omega \simeq V_0 \alpha^{2/3} \quad (\alpha \gg 1) . \]

These expressions show that the tunneling frequency \( \Omega \) can be regulated, by changing \( r_0 \) and \( V_0 \), in a wide range \( 0 < \Omega < \infty \). This means that varying the shape of the double-well potential, which is achievable in experiments [16–21], one can regulate the tunneling properties of the system.

### III Equilibrium Phases

Thermodynamics of the system with Hamiltonian (20), for sufficiently long-range interactions, can be accurately described in the mean-field approximation [37] corresponding
to the equality
\[ S^\alpha_i S^\beta_j = < S^\alpha_i > S^\beta_j + S^\alpha_i < S^\beta_j > - < S^\alpha_i > < S^\beta_j > \quad (i \neq j), \tag{21} \]
where the angle brackets imply statistical averaging. We introduce the notation for the average interaction strengths
\[ A \equiv \frac{1}{N_L} \sum_{i \neq j} A_{ij}, \quad B \equiv \frac{1}{N_L} \sum_{i \neq j} B_{ij}, \quad I \equiv \frac{1}{N_L} \sum_{i \neq j} I_{ij}. \tag{22} \]
Also, we define the effective tunneling frequency
\[ \Omega_{\text{eff}} \equiv \Omega - 2B < S^x_j > \tag{23} \]
and the effective mean field
\[ h_{\text{eff}} \equiv \sqrt{\Omega_{\text{eff}}^2 + 4I^2 < S^z_j >^2}. \tag{24} \]

Using the standard methods of dealing with pseudospin Hamiltonians [38], we find
\[ < S^x_j > = \frac{\Omega_{\text{eff}}}{2h_{\text{eff}}} \tanh \left( \frac{h_{\text{eff}}}{2T} \right), \quad < S^y_j > = 0, \]
\[ < S^z_j > = < S^z_j > \frac{I}{h_{\text{eff}}} \tanh \left( \frac{h_{\text{eff}}}{2T} \right), \tag{25} \]
where \( T \) is temperature. The system free energy reads as
\[ F = NE_0 + \frac{N}{2} \left( A - 2B < S^x_j >^2 + 2I < S^z_j >^2 \right) - NT \ln \left( 2\cosh \frac{h_{\text{eff}}}{2T} \right), \tag{26} \]
in which \( N = N_L \) because of the unity filling factor. From the latter equation, one can calculate all thermodynamics characteristics.

We shall be mainly interested in the properties of the average tunneling intensity
\[ x \equiv \frac{2}{N_L} \sum_j < S^x_j >, \tag{27} \]
average Josephson current
\[ y \equiv \frac{2}{N_L} \sum_j < S^y_j >, \tag{28} \]
and the average well imbalance
\[ z \equiv \frac{2}{N_L} \sum_j < S^z_j >. \tag{29} \]

The properties of the system depend on the parameters defined in Eq. (22), which characterize the effective interaction strength. The parameter \( A \) enters the free energy (26) additively, hence, it does not play here an important role. The parameter \( B \) is...
composed of the effective interactions $B_{ij}$ given in Eq. (14). The symmetric terms $V_{ij}^{1111}$, $V_{ij}^{2222}$, and $V_{ij}^{1221}$ are close to each other, because of which the transverse interactions $B_{ij}$ are small, so that the parameter $B$ is substantially smaller than the parameter $I$. The main role among interactions is played by the longitudinal interaction strength $I$. Here we assume that $I$ is positive, which is the often situation for the exchange interactions \cite{30,37,38}. Then, as follows from Hamiltonian (20), the nearest spins $S_i^z$ and $S_j^z$ tend to align parallel in order to reduce the system energy. Therefore only the ferromagnetic-type order is possible in the system \cite{30,37,38}.

Generally, the exchange interactions $I_{ij}$ could be negative. Then the longitudinal term in Hamiltonian (20) would enter with the sign plus, which would imply that the nearest spins prefer to align antiparallel to each other in order to lower the system energy. In that case, the antiferromagnetic-type order could be the sole possibility. In the present paper, we limit the consideration by a positive parameter $I > 0$, which means that only a ferromagnetic-type order can arise.

To simplify the formulas, we use the dimensionless quantities, such as the dimensionless tunneling frequency

$$\omega \equiv \frac{\Omega}{I + B},$$

and the dimensionless transverse interaction

$$b \equiv \frac{B}{I + B}.$$  \hspace{1cm} (31)

Also, we define the dimensionless field

$$h \equiv \frac{h_{\text{eff}}}{I + B},$$

which, with the use of the above notations, becomes

$$h = \sqrt{(\omega - bx)^2 + (1 - b)^2 z^2}.$$  \hspace{1cm} (33)

From definitions (27) to (29) and Eqs. (25), we have the tunneling intensity

$$x = \frac{\omega - bx}{h} \tanh \left( \frac{h}{2T} \right),$$

Josephson current in equilibrium

$$y = 0,$$  \hspace{1cm} (35)

and the well imbalance

$$z = z \frac{1 - b}{h} \tanh \left( \frac{h}{2T} \right),$$

where temperature $T$ is measured in units of $I + B$.

We may notice that Eqs. (34) to (36) are invariant under the replacement

$$x \rightarrow -x, \quad \omega \rightarrow -\omega, \quad z \rightarrow -z.$$  \hspace{1cm} (37)

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Therefore, without the loss of generality, we can consider only the case with $x \geq 0$, $\omega \geq 0$, and $z \geq 0$.

Equation (36) shows that there can exist two thermodynamic phases, ordered and disordered, when, respectively,

$$z \neq 0 \quad (ordered) ,$$

$$z = 0 \quad (disordered) .$$

In the ordered phase, the mean well imbalance is nonzero, and one has

$$x = \omega \quad (z \neq 0) ,$$

with $z$ given by the equation

$$\frac{1 - b}{h} \tanh \left( \frac{h}{2T} \right) = 1 .$$

From Eqs. (33) and (38), it follows that

$$h = (1 - b) \sqrt{\omega^2 + z^2} .$$

The ordered phase exists, when two conditions are valid, the tunneling frequency is not too high,

$$0 \leq \omega < 1 ,$$

and the temperature is lower than the critical temperature

$$T_c = \frac{(1 - b)\omega}{2 \text{artanh } \omega} ,$$

so that

$$0 \leq T < T_c .$$

When at least one of conditions (40) or (42) is not valid, that is, either $\omega \geq 1$ or $T \geq T_c$, the ordered phase cannot exist and transfers to the disordered phase.

In the disordered phase, the mean well imbalance is zero, and one has

$$x = \tanh \left( \frac{\omega - bx}{2T} \right) \quad (z = 0) ,$$

which defines the tunneling intensity $x$.

At zero temperature $T = 0$, the ordered phase is described by the equations

$$x = \omega , \quad z = \sqrt{1 - \omega^2} \quad (\omega < 1) .$$

While the disordered phase is characterized by the expressions

$$x = 1 , \quad z = 0 \quad (\omega > 1) .$$

The quantum phase transition between the ordered and disordered phases occurs at the tunneling frequency $\omega = 1$.
IV  Collective Excitations

Collective excitations in the system represented by the pseudospin Hamiltonian (20), correspond to pseudospin waves. The Heisenberg equations of motion for the pseudospin operators yield

\[
\frac{dS_i^x}{dt} = 2S_i^y \sum_{j(\neq i)} I_{ij} S_j^z ,
\]

\[
\frac{dS_i^y}{dt} = \Omega S_i^z - 2S_i^z \sum_{j(\neq i)} I_{ij} S_j^z - 2S_i^z \sum_{j(\neq i)} B_{ij} S_j^x ,
\]

\[
\frac{dS_i^z}{dt} = -\Omega S_i^y + 2S_i^y \sum_{j(\neq i)} B_{ij} S_j^x .
\]  \hspace{1cm} (46)

For describing collective excitations, we employ the Fourier transformation for the pseudospin operators

\[
S_j^\alpha = \frac{1}{N_L} \sum_k \sigma_k^\alpha e^{i k \cdot a_j} , \quad \sigma_k^\alpha = \sum_j S_j^\alpha e^{-i k \cdot a_j} ,
\]  \hspace{1cm} (47)

where \( k \) pertains to the first Brillouin zone. Similarly, we expand the interaction functions

\[
I_{ij} = \frac{1}{N_L} \sum_k I_k e^{i k \cdot a_{ij}} , \quad B_{ij} = \frac{1}{N_L} \sum_k B_k e^{i k \cdot a_{ij}} ,
\]  \hspace{1cm} (48)

in which \( a_{ij} = a_i - a_j \). Then, Eqs. (46) acquire the form

\[
\frac{d\sigma_k^x}{dt} = \frac{2}{N_L} \sum_p I_{k-p} \sigma_p^y \sigma_{k-p}^z ,
\]

\[
\frac{d\sigma_k^y}{dt} = \Omega \sigma_k^z - \frac{2}{N_L} \sum_p I_{k-p} \sigma_p^y \sigma_{k-p}^z - \frac{2}{N_L} \sum_p B_{k-p} \sigma_p^x \sigma_{k-p}^z ,
\]

\[
\frac{d\sigma_k^z}{dt} = -\Omega \sigma_k^y + \frac{2}{N_L} \sum_p B_{k-p} \sigma_p^y \sigma_{k-p}^x ,
\]  \hspace{1cm} (49)

where \( \sigma_k^\alpha = \sigma_k^\alpha(t) \).

To find the spectrum of collective excitations, we resort to the random-phase approximation. For this purpose, we look for the solutions to Eqs. (49) in the form

\[
\sigma_k^\alpha(t) = < \sigma_k^\alpha > + \delta \sigma_k^\alpha e^{-i \epsilon t} ,
\]  \hspace{1cm} (50)

describing the deviations from the equilibrium values

\[
< \sigma_k^\alpha > = \delta_{k0} N_L < S_j^\alpha > .
\]

Linearizing Eqs. (49) with respect to \( \delta \sigma_k^\alpha \) yields for the spectrum of pseudospin waves

\[
\epsilon_k^2 = (\Omega - Bx)[\Omega - (B + I_k)x] + I(I + B_k)z^2 .
\]  \hspace{1cm} (51)
In deriving Eq. (51), we have taken into account that
\[
\lim_{k \to 0} I_k = I , \quad \lim_{k \to 0} B_k = B ,
\]
with \( I \) and \( B \) defined in Eq. (22).

To consider the spectrum property in the long-wave limit, we use the asymptotic equalities
\[
I_k \simeq I - \frac{1}{2} \sum_i I_{ij} (k \cdot a_{ij})^2 , \quad B_k \simeq B - \frac{1}{2} \sum_i B_{ij} (k \cdot a_{ij})^2 , \tag{52}
\]
where \( k \to 0 \). We define the gap \( \Delta \) by the equation
\[
\left( \frac{\Delta}{I + B} \right)^2 = (\omega - bx)(\omega - x) + (1 - b)z^2 . \tag{53}
\]
And let us introduce a matrix \( G_{ij} \), given by the equality
\[
\frac{G_{ij}}{I + B} = (\omega - bx)xI_{ij} - (1 - b)z^2 B_{ij} . \tag{54}
\]
Then the long-wave limit of spectrum in Eq. (51) gives
\[
\varepsilon_k^2 \simeq \Delta^2 + \frac{1}{2} \sum_i G_{ij} (k \cdot a_{ij})^2 . \tag{55}
\]
The spectrum is quadratic, which is typical of spin waves.

Specifying the gap \( \Delta \) and the matrix \( G_{ij} \) for the ordered and disordered phases, we have for the ordered phase, when \( z \neq 0 \),
\[
\frac{\Delta}{I + B} = \sqrt{1 - b} z , \quad \frac{G_{ij}}{I + B} = (1 - b) \left( \omega^2 I_{ij} - z^2 B_{ij} \right) ,
\]
and for the disordered phase, with \( z = 0 \),
\[
\frac{\Delta}{I + B} = \sqrt{(\omega - bx)(\omega - x)} , \quad \frac{G_{ij}}{I + B} = (\omega - bx)xI_{ij} .
\]
The gap disappears at the critical point of the order-disorder phase transition. Approaching this point from the side of the ordered phase, one has \( z \to 0 \), while approaching the point from the side of the disordered phase, one has \( x \to \omega \). In both these cases, \( \Delta \to 0 \) at the critical point.

**V  Nonequilibrium Loading**

Let us suppose that atoms are loaded into a double-well lattice in an initially nonequilibrium state. For describing their equilibration process, one needs to study the temporal behavior of the variables defined in Eqs. (27) to (29) and characterizing the tunneling
intensity $x = x(t)$, Josephson current $y = y(t)$, and the well imbalance $z = z(t)$. The evolution equations for these quantities can be obtained by averaging the operator equations (46). For this purpose, one often employs the mean-field approximation. This approximation does not take into account the relaxation processes due to atomic interactions. However, such processes could be important in order that equilibrium would be possible. Therefore, we shall resort to a more accurate approximation, called the local-field approximation. This approximation, suggested by Wangness [39], treats atomic interactions as occurring in a local field formed by other particles, which results in the appearance of relaxation characterized by the attenuation parameters, $\gamma_1$ and $\gamma_2$ whose values can be calculated through the given atomic interactions. The local-field approximation assumes the existence of local equilibrium [40], so that at each moment of time the variables tend to relax to the locally-equilibrium state. Averaging Eqs. (46) in the frame of the local-field approximation [39] yields the system of equations

$$
\frac{dx}{dt} = (1 - b)yz - \gamma_2(x - x_t), \quad \frac{dy}{dt} = (\omega - x)z - \gamma_2(y - y_t),
$$

$$
\frac{dz}{dt} = (bx - \omega)y - \gamma_1(z - z_t),
$$

(56)

where the time variable is measured in units of $1/(I + B)$, while the attenuation parameters $\gamma_1$ and $\gamma_2$, in units of $I + B$, and the local fields are

$$
x_t = \frac{\omega - bx}{h} \tanh \left( \frac{h}{2T} \right), \quad y_t = 0,
$$

$$
z_t = \frac{1 - b}{h} z \tanh \left( \frac{h}{2T} \right).
$$

(57)

Here $T$ is the temperature, in units of $I + B$, corresponding to a would be equilibrium state, the type of the latter being defined by the system parameters. The explicit expression for $h$ is given in Eq. (33). The evolution equations (56) are supplemented with the initial conditions

$$
x(0) = x_0, \quad y(0) = y_0, \quad z(0) = z_0,
$$

(58)

which, generally, represent a nonequilibrium state.

Keeping in mind applications to ultracold atoms, we may set temperature to zero. Then, Eqs. (56) possess two types of stationary solutions. One type is defined by the fixed point

$$
x^*_1 = \omega, \quad y^*_1 = 0, \quad z^*_1 = \sqrt{1 - \omega^2},
$$

(59)

which corresponds to the ordered phase. While another type is given by the fixed point

$$
x^*_2 = 1, \quad y^*_2 = 0, \quad z^*_2 = 0,
$$

(60)

corresponding to the disordered phase. The question remains whether an atomic system loaded into the double-well lattice, in an initially nonequilibrium state, would relax to one of the stationary solutions.
VI Stability Analysis

The stability of stationary solutions can be studied by the Lyapunov stability analysis. To this end, we calculate, in the standard way, the Jacobian matrix associated with the dynamical system (56). Then we find the eigenvalues of the Jacobian matrix, denoted by $\lambda$, which give the characteristic exponents. The real parts $\text{Re} \, \lambda$ define the Lyapunov exponents describing the stability properties. For simplicity, we set $\gamma_1 = \gamma_2 = \gamma$.

Accomplishing this procedure for the fixed point (59), we find that it is stable when $\omega < 1$. One of the characteristic exponents is exactly

$$
\lambda_1 = -\gamma .
$$

(61)

The expressions for two other characteristic exponents are rather cumbersome, because of which we write them down to the first order in $\gamma$, resulting in

$$
\lambda_{2,3} \simeq - \frac{2 - b - \omega^2}{2(1 - b)} \gamma \pm i\omega_{\text{eff}} ,
$$

(62)

with the effective frequency

$$
\omega_{\text{eff}} = \sqrt{(1 - b)(1 - \omega^2)} \quad (\omega < 1) .
$$

(63)

This shows that the fixed point (59) is a stable focus, when $\omega < 1$ and $\gamma$ is small. Recall that by its definition (31), one always has $b < 1$.

The fixed point (60) is stable for $\omega > 1$. Then, one of the characteristic exponents is exactly the same as Eq. (61). Two other characteristic exponents, to the first order in $\gamma$, are

$$
\lambda_{2,3} \simeq - \frac{2\omega - 1 - b}{2(\omega - b)} \gamma \pm i\omega'_{\text{eff}} ,
$$

(64)

with the effective frequency

$$
\omega'_{\text{eff}} = \sqrt{(\omega - 1)(\omega - b)} \quad (\omega > 1) .
$$

(65)

Thus, the fixed point (60) is also a stable focus for $\omega > 1$ and small $\gamma$.

The value of the tunneling frequency $\omega = 1$ is a bifurcation point related to the dynamical phase transition. At this point, the dynamical system is neutral, with the characteristic exponents

$$
\lambda_1 = -\gamma , \quad \lambda_2 = 0 , \quad \lambda_3 = -\gamma \quad (\omega = 1)
$$

for any $\gamma$.

An important observation, following from the above analysis, is that the dynamical system is structurally stable only in the presence of the damping parameter $\gamma > 0$. Setting the latter to zero leads to the characteristic exponents for the ordered fixed point (59)

$$
\lambda_1 = 0 , \quad \lambda_{2,3} = \pm i\omega_{\text{eff}} \quad (\gamma = 0, \, \omega < 1)
$$

for any $\gamma$.
and for the disordered fixed point (60)

$$\lambda_1 = 0, \quad \lambda_{2,3} = \pm i \omega'_{\text{eff}} \quad (\gamma = 0, \, \omega > 1)$$

where $\omega_{\text{eff}}$ and $\omega'_{\text{eff}}$ are given by Eqs. (63) and (65). These characteristic exponents demonstrate that the dynamical system is structurally unstable.

But the case of no attenuation corresponds to the usual mean-field approximation. Hence the above consideration shows that the mean-field approximation results in a structurally unstable dynamical system, thus, this approximation cannot correctly describe the evolutional processes of atoms in a double-well lattice.

In order to illustrate in an explicit way the difference between the temporal behavior of solutions to the evolution equations (56) and the related mean-field approximations, with no attenuation, we solve Eqs. (56) numerically. The initial conditions (58) are chosen so that to correspond to an initially nonequilibrium state.

In Fig. 1, the relaxation to the ordered stationary solution (59) is shown for $\gamma = 1$ and $\omega < 1$. Taking the attenuation parameter $\gamma$ equal to one in dimensionless units implies that it is of order $I + B$ in dimensional units. For these parameters, the fixed point (59) becomes a stable node. Contrary to this, the mean-field approximation, with $\gamma = 0$, exhibits permanently oscillating solutions. The curves for $x(t)$ and $z(t)$ always oscillate around the given initial conditions, which is not a correct behavior. In turn, the latter is caused by the structural instability of the dynamical system in the mean-field approximation. The relaxation to the disordered stationary solution (60) is demonstrated in Fig. 2 for $\omega > 1$ and $\gamma = 1$, when Eq. (60) corresponds to a stable node. But the mean-field approximation, with $\gamma = 0$, again exhibits an incorrect oscillatory behavior depending on the choice of the initial conditions (58). Again, it is the structural instability that is responsible for the incorrect dynamics in the mean-field approximation.

Full equations (56) can also exhibit the oscillatory behavior of their solutions. This happens when the fixed points are the stable foci, which occurs for $\gamma \ll \omega$, as follows from Eqs. (62) to (65). In particular, if $\omega \gg 1$, than, according to Eq. (65), the oscillation period approximately is $2\pi/\omega$. This situation is illustrated in Fig. 3.

**VII Discussion**

We have considered a system of atoms in a double-well optical lattice. The case of an insulating lattice with the unity filling factor is studied. This type of double-well optical lattices is of special interest, being a convenient setup for realizing the ordered and disordered states of atoms in a double-well lattice.

The principal difference of the present paper, as compared to the earlier theoretical works on the double-well lattices [22–24, 41], where the superfluidity-insulator phase transition is studied for atoms with local interactions, is that we consider an insulating double-well lattice, with atoms possessing long-range interactions. An effective Hamiltonian in the pseudospin representation is derived. The system exhibits two thermodynamic phases, ordered and disordered. The phase transition between the phases can be driven either by temperature or by varying the system parameters. For instance, one can vary the strength of atomic interactions or the shape of the double-well potential.
The spectrum of collective excitations has the form typical of that for pseudospin waves. In the long-wave limit, the spectrum is quadratic, with a gap. The latter disappears at the phase transition point.

Nonequilibrium properties of the system are investigated. Physically, the situation can correspond to atoms loaded into a lattice in an initially nonequilibrium state. Such a nonequilibrium state can also be prepared by disturbing the lattice by external fields.

The relaxation of the system, from an initially nonequilibrium state to equilibrium, cannot be described by the mean-field approximation. This is rather clear from the physical point of view, since the mean-field approximation does not take into account attenuation effects, hence, is not able to describe the equilibration process in principle.

From the mathematical point of view, as we show, the mean-field approximation results in a structurally unstable dynamical system. To correctly describe the process of relaxation, the damping effects, caused by atomic interactions, must be included. This can be done, e.g., by employing the local-field approximation.

The long-range interactions that would be sufficient for realizing the effects described above could be of dipolar type, such as occur for polar molecules [31,42], Rydberg atoms [32], and quantum gases with dipolar atomic interactions (see review articles [33,43]). A good candidate would be the gas of cold atoms $^{52}$Cr, possessing large magnetic moment of $6\mu_B$ and, as a result, sufficiently strong dipolar interactions [44,45]. Because of the existence of several species exhibiting long-range dipolar interactions, the latter can be of different strength. In addition, these interactions can be effectively modulated by external magnetic or electric fields, thus, tuning the interaction strength in a wide range [46–49].

In the dynamics of atoms, relaxing from a nonequilibrium state to their equilibrium, an important role is played by the attenuation parameter $\gamma$. The calculation of the latter, for systems with dipolar interactions, is a well known procedure, described in detail in literature on magnetic resonance [50–55]. In the case of particles with magnetic moment $\mu$, interacting through magnetic dipolar forces, an accurate value of the attenuation parameter is given by the expression $\gamma = \rho z_0 \mu^2 / \hbar$, where $\rho$ is the mean particle density and $z_0$ is the number of nearest neighbors. This value of $\gamma$ is of the order of the interaction strength. That is why setting, in dimensionless units, $\gamma$ to one, as we have done in numerical calculations, is absolutely natural.

Taking, for illustration, the magnetic moment of $^{52}$Cr, equal to $\mu = 6\mu_B$, with $\mu_B = 0.927 \times 10^{-20}$ erg/G being the Bohr magneton, the typical atomic densities in a trap $\rho \sim (10^{12} - 10^{15})$ cm$^{-3}$, and accepting for the number of nearest neighbors $z_0 \sim 10$, we have $\gamma \sim (1 - 10^3)$ s$^{-1}$. This means that the relaxation time $T_{rel} \equiv 1/\gamma$ is of order $T_{rel} \sim (10^{-3} - 1)$ s. The lifetime of trapped atomic systems can vary in the range of $t_{exp} \sim (1 - 100)$ s. Therefore, the relaxation time $T_{rel}$ in many cases is much smaller than $t_{exp}$, which implies that taking into account the attenuation is of critical importance. The simple mean-field approximation without taking account of the relaxation effects would be qualitatively incorrect.

In conclusion, it is worth noting that the shape of the double-well potential can be easily regulated. Hence, it is possible to organize any required sequence of transitions between the ordered and disordered states in the double-well lattice during the system lifetime.
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Appendix A

The eigenproblem for the lattice Hamiltonian (2),

\[ H_L(r) \varphi_{nk}(r) = E_{nk} \varphi_{nk}(r) , \]
defines the Bloch functions \( \varphi_{nk}(r) \) and the Bloch spectrum \( E_{nk} \). This eigenproblem, invoking the relation between the Bloch and Wannier functions

\[ \varphi_{nk}(r) = \frac{1}{\sqrt{N_L}} \sum_j w_n(r - a_j) e^{i \mathbf{k} \cdot a_j} , \]
can be rewritten as

\[ H_L(r) w_n(r - a_j) = \frac{1}{N_L} \sum_{ik} E_{nk} e^{i \mathbf{k} \cdot a_{ij}} w_n(r - a_i) , \]
where \( a_{ij} \equiv a_i - a_j \). Using this in Eq. (5) gives Eq. (6), with

\[ E_{ij}^n = \frac{1}{N_L} \sum_k E_{nk} e^{i \mathbf{k} \cdot a_{ij}} . \]
Representing the latter in form (7) yields

\[ E_n = \frac{1}{N_L} \sum_k E_{nk} \]
and

\[ J_{ij}^n = \frac{1}{N_L} \sum_k E_{nk} e^{i \mathbf{k} \cdot a_{ij}} \quad (i \neq j) . \]
These properties are used in deriving Hamiltonian (10).
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Figure Captions

**Fig. 1.** Dimensionless variables describing the tunneling intensity $x(t)$, Josephson current $y(t)$, and well population imbalance $z(t)$ as functions of dimensionless time for $\omega = 0.1$ and $b = 0.5$. Initial conditions are $x_0 = 0.66$, $y_0 = 0.75$, and $z_0 = 0$. The case of no attenuation ($\gamma = 0$) is shown by the dashed curve. The case with attenuation ($\gamma = 1$) is represented by the solid line.

**Fig. 2.** Dimensionless variables $x(t)$, $y(t)$, and $z(t)$ as functions of dimensionless time for $\omega = 1.5$ and $b = 0.5$. Initial conditions are $x_0 = 0.33$, $y_0 = 0.5$, and $z_0 = 0.8$. The attenuation parameters are: $\gamma = 0$ (dashed line) and $\gamma = 1$ (solid line).

**Fig. 3.** Population imbalance for large tunneling $\omega = 100$, with $\gamma = 1$ and $b = 0.5$ as a function of dimensionless time. Initial conditions are $x_0 = 0$, $y_0 = 0$, and $z_0 = 1$. 
Figure 1: Dimensionless variables describing the tunneling intensity $x(t)$, Josephson current $y(t)$, and well population imbalance $z(t)$ as functions of dimensionless time for $\omega = 0.1$ and $b = 0.5$. Initial conditions are $x_0 = 0.66$, $y_0 = 0.75$, and $z_0 = 0$. The case of no attenuation ($\gamma = 0$) is shown by the dashed curve. The case with attenuation ($\gamma = 1$) is represented by the solid line.
Figure 2: Dimensionless variables $x(t)$, $y(t)$, and $z(t)$ as functions of dimensionless time for $\omega = 1.5$ and $b = 0.5$. Initial conditions are $x_0 = 0.33$, $y_0 = 0.5$, and $z_0 = 0.8$. The attenuation parameters are: $\gamma = 0$ (dashed line) and $\gamma = 1$ (solid line).
Figure 3: Population imbalance for large tunneling $\omega = 100$, with $\gamma = 1$ and $b = 0.5$ as a function of dimensionless time. Initial conditions are $x_0 = 0$, $y_0 = 0$, and $z_0 = 1$. 