Abstract: An ultracold gas is considered, loaded into a lattice, each site of which is formed by a double-well potential. Initial conditions, after the loading, correspond to a nonequilibrium state. The nonlinear dynamics of the system, starting with a nonequilibrium state, is analysed in the local-field approximation. The importance of taking into account attenuation, caused by particle collisions, is emphasized. The presence of this attenuation dramatically influences the system dynamics.

Nonlinear dynamics of ultracold gases in double-well lattices

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1. Introduction

Present-day experiments provide the possibility of creating a large variety of optical and magnetic lattices with loaded ultracold Bose and Fermi gases [1–6]. One of the main advantages of such systems is the potentialities of their almost complete control. The parameters of the lattices themselves can be varied in a wide range, as well as there exists a great diversity of characteristics of ultracold gases, both Bose [7–13] as well as Fermi [14–16]. Such a high level of control suggests the feasibility of numerous applications. For many of these applications, it is important to have a correct description of the system dynamic properties.

Recently, the variety of lattices has been expanded with the experimental realization of double-well optical lattices, each site of such lattices being formed by a double-well optical potential [17]. Such more complicated double-well lattices possess a rich variety of thermodynamic equilibrium states [18]. Dynamics of atoms in these complex lattices should also be more rich, presenting novel possibilities that could be employed for various practical purposes, for instance, in quantum information processing and quantum computing.

Atomic dynamics inside a separate double-well have been studied earlier [19–21]. The aim of the present paper is to analyze dynamics not inside a separate double-well, but in the whole double-well lattice, composed of many double-well sites.

We consider atoms in a double-well lattice, which in equilibrium would form the Mott insulating state. But initially atoms are loaded in a nonequilibrium state. Describing their dynamics, it is important to invoke realistic ap-
proximations, taking into account attenuation caused by atomic collisions. Resorting to a simple mean-field approximation, usually employed for treating atomic dynamics inside a separate double well, would result in perpetual oscillations, never coming to a stationary state corresponding to equilibrium. Therefore, including attenuation is of crucial importance.

The plan of the present paper is as follows. First, we derive the effective Hamiltonian for ultracold gases in an insulating double-well lattice (Sec. 2). Then we consider the nonlinear evolution equations, taking account of particle interactions and attenuation, for the dynamic variables describing particle tunneling, Josephson current, and atomic displacements (Sec. 3). In Sec. 4, we investigate the existence and stability of attractors, and present the results of numerical calculations. Finally, Sec. 5 is conclusion.

2. Effective Hamiltonian

The starting point is the standard energy Hamiltonian in the Heisenberg field representation,

\[ H = \int \psi^\dagger(r) H_L(r) \psi(r) \, dr + \frac{1}{2} \int \psi^\dagger(r) \psi^\dagger(r') \phi(r-r') \psi(r') \psi(r) \, dr \, dr', \]

in which \( \psi(r) \) is a field operator, where the time dependence, for brevity, is omitted, but keeping in mind that \( \psi(r) \equiv \psi(r, t) \) is the Heisenberg field operator; \( \phi(r) = \phi(-r) \) is an interaction potential; and

\[ H_L(r) = -\nabla^2 r + V_L(r), \]

where the lattice potential \( V_L(r) \) is assumed to have the double-well structure in each lattice site marked by a lattice vector \( a_i \). For generality, we do not specify a particular form of the interaction potential \( \phi(r) \), since in experiments it can have different forms. It can be a local potential [7–11], or a long-range dipolar potential, or a combination of a contact and dipolar potentials [22]. The strength of atomic interactions can also be varied in a very wide range by using Feshbach resonance techniques [23,24].

The lattice is assumed to be sufficiently deep in order to realize the Mott insulating state, when the wave functions \( \varphi_n(r - a_i) \), which are the solutions of the eigenproblem

\[ H_L(r-a_i) \varphi_n(r-a_i) = E_n \varphi_n(r-a_i), \]

are well localized around the related lattice sites \( a_i \). Then the jumps of atoms between different sites are suppressed, as it should be for an insulating state. However the tunneling between the wells of a double-well potential, associated to each lattice site, can be arbitrary and can be regulated by varying the shape of the double well [25].

Expanding the field operator as

\[ \psi(r) = \sum_{i,n} c_{in} \varphi_n(r - a_i), \]

we can transform Hamiltonian (1) to the representation of operators \( c_{in} \), whose commutation relations are prescribed by the sort of atoms, which can be either bosons or fermions. In an insulating state, the filling factor is to be integer, which we set to one. This implies the homeopolarity conditions

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

Substituting expansion (4) into Hamiltonian (1) and retaining overlaps up to second order, gives

\[ \hat{H} = \sum_{i,n} E_n c_{in}^\dagger c_{in} + \frac{1}{2} \sum_{i \neq j} \sum_{m,n,m',n'} V_{ij}^{mn,m'n'} c_{im}^\dagger c_{jn}^\dagger c_{jm} c_{in}, \]

where

\[ V_{ij}^{mn,m'n'} \equiv \delta_{ij} \delta_{jj} \delta_{mm'} + \delta_{mm} \delta_{jj} - \delta_{ij} \delta_{jj} \delta_{mn} \]

is expressed through the matrix elements of the interaction potential with respect to the wave functions \( \varphi_n(r - a_i) \).

The system temperature is assumed to be close to zero, so that, of the double-well spectrum, only two lowest energy levels may be taken into account. These levels, \( E_1 \) and \( E_2 \), are enumerated with the index \( n = 1 \) and \( n = 2 \). The wave functions of the lowest levels, corresponding to a double-well potential, are such that the ground-state function is symmetric with respect to spatial inversion, while the first excited state is antisymmetric [25],

\[ \varphi_1(-r) = \varphi_1(r), \quad \varphi_2(-r) = -\varphi_2(r). \]

Both functions \( \varphi_1(r) \) and \( \varphi_2(r) \) are real.

By introducing the pseudospin operators

\[ S_i^x = \frac{1}{2} (c_{i1}^\dagger c_{i2} - c_{i2}^\dagger c_{i1}), \quad S_i^y = \frac{i}{2} (c_{i1}^\dagger c_{i2} - c_{i2}^\dagger c_{i1}), \quad S_i^z = \frac{1}{2} (c_{i1}^\dagger c_{i2} + c_{i2}^\dagger c_{i1}), \]

we have

\[ c_{i1}^\dagger c_{i2} = \frac{1}{2} + S_i^x, \quad c_{i2}^\dagger c_{i1} = \frac{1}{2} - S_i^x, \quad c_{i1}^\dagger c_{i1} = \frac{1}{2} + S_i^y, \quad c_{i2}^\dagger c_{i2} = \frac{1}{2} - S_i^y. \]

In order to better understand the meaning of the pseudospin operators (8), we may define the left, \( c_{iL} \), and the right, \( c_{iR} \), operators by the relations

\[ c_{i1} = \frac{1}{\sqrt{2}} (c_{iL} + c_{iR}), \quad c_{i2} = \frac{1}{\sqrt{2}} (c_{iL} - c_{iR}). \]
Then the operators (8) acquire the form
\[
S_i^x = \frac{1}{2} (c_{iL}^\dagger c_{iR} + c_{iR}^\dagger c_{iL}), \quad (11)
\]
\[
S_i^y = -\frac{i}{2} (c_{iL}^\dagger c_{iR} - c_{iR}^\dagger c_{iL}), \quad (12)
\]
\[
S_i^z = \frac{1}{2} (c_{iL}^\dagger c_{iL} - c_{iR}^\dagger c_{iR}).
\]
From here, we see that \( S_i^z \) describes the tunneling intensity between the left and right wells of a double-well potential located at the \( i \)-site. The operator \( S_i^y \) characterizes the Josephson current between the left and right wells. And \( S_i^x \) is a displacement operator showing the imbalance between the wells.

Let us introduce the notation
\[
E_0 \equiv \frac{1}{2} (E_1 + E_2)
\]
and define the following combinations of the interaction matrix elements
\[
A_{ij} \equiv \frac{1}{2} (V_{ij}^{1111} + V_{ij}^{2222} + 2V_{ij}^{1221}), \quad (13)
\]
\[
B_{ij} \equiv \frac{1}{2} (V_{ij}^{1111} + V_{ij}^{2222} - 2V_{ij}^{1221}), \quad (14)
\]
\[
C_{ij} \equiv \frac{1}{2} (V_{ij}^{2222} - V_{ij}^{1111}), \quad J_{ij} \equiv -2V_{ij}^{1122}.
\]
Also, we define the tunneling parameter
\[
\Omega \equiv E_2 - E_1 + \sum_{j \neq i} C_{ij}.
\]
Then Hamiltonian (6) reduces to the effective pseudospin representation
\[
\hat{H} = E_0 N + \frac{1}{2} \sum_{i \neq j} A_{ij} - \Omega \sum_i S_i^z + \sum_{i \neq j} B_{ij} S_i^z S_j^z - \sum_{i \neq j} J_{ij} S_i^z S_j^z,
\]
in which \( N \) is the number of atoms in the lattice.

3. Evolution equations

The Heisenberg equations of motion for operators (8) are
\[
\frac{dS_i^x}{dt} = 2S_i^y \sum_{j \neq i} J_{ij} S_j^z, \quad (16)
\]
\[
\frac{dS_i^y}{dt} = \Omega S_i^z - 2S_i^x \sum_{j \neq i} J_{ij} S_j^z - 2S_i^z \sum_{j \neq i} B_{ij} S_j^z, \quad (17)
\]
\[
\frac{dS_i^z}{dt} = -\Omega S_i^z + 2S_i^x \sum_{j \neq i} B_{ij} S_j^z.
\]
Our aim is to study the evolution of the averages
\[
x = \frac{2}{N} \sum_i \langle S_i^x \rangle, \quad (18)
\]
\[
y = \frac{2}{N} \sum_i \langle S_i^y \rangle, \quad (19)
\]
\[
z = \frac{2}{N} \sum_i \langle S_i^z \rangle,
\]
describing the temporal behavior of the tunneling intensity \( x = x(t) \), Josephson current \( y = y(t) \), and the imbalance variable \( z = z(t) \).

Considering the statistical averaging in Eq. (16), we need to choose a decoupling for the pair correlators of spin operators. The simplest option, which is usually accepted, would be the mean-field, or semiclassical, approximation, neglecting all pair correlations. Such a semiclassical approximation does not take into account quantum effects, due to particle collisions, which cause the attenuation of dynamical variables.

To take into account such damping effects, we can employ the local-field approximation that is used in the theory of magnetic resonance [26,27] and in the calculations of the dielectric response functions [28]. The idea of this approximation is the existence of a kind of local equilibrium even in strongly nonequilibrium systems [29,30]. Particle collisions are considered as occurring in an effective local field of other particles [26]. Technically, for the system we consider here, the local-field approximation is realized as follows. First, one considers equilibrium mean-field solutions for Hamiltonian (15). Then, introducing the notation
\[
J \equiv \frac{1}{N} \sum_{i \neq j} J_{ij}, \quad B \equiv \frac{1}{N} \sum_{i \neq j} B_{ij},
\]
we have
\[
\langle S_i^x \rangle = \frac{\Omega - 2B \langle S_i^z \rangle}{2D} \tanh \left( \frac{D}{2T} \right), \quad (19)
\]
\[
\langle S_i^y \rangle = 0, \quad \langle S_i^z \rangle = \frac{J \langle S_i^z \rangle}{D} \tanh \left( \frac{D}{2T} \right),
\]
where \( T \) is temperature and
\[
D \equiv \sqrt{(\Omega - 2B \langle S_i^z \rangle)^2 + 4J^2 \langle S_i^z \rangle^2}.
\]
The same form of solutions (19) is assumed to hold locally in time and space, when the system is in local equilibrium. This means that, in local equilibrium, the average variables (17) are of the form
\[
x_t = \frac{\Omega - Bx}{D_t} \tanh \left( \frac{D_t}{2T} \right), \quad (20)
\]
\[
y_t = 0, \quad z_t = \frac{Jz}{D_t} \tanh \left( \frac{D_t}{2T} \right),
\]
in which
\[
D_t \equiv \sqrt{(\Omega - Bx)^2 + J^2z^2}.\]
The evolution equations for variables (17) are obtained by averaging Eq. (16), decoupling the pair spin correlations, but including the damping, caused by particle collisions, so that the variables would attenuate to their local forms (20). This procedure yields the evolution equations

\[
\frac{dx}{dt} = Jyz - \gamma_2(x - x_t),
\]

\[
\frac{dy}{dt} = \Omega z - (J + B)xz - \gamma_2(y - y_t),
\]

\[
\frac{dz}{dt} = -\Omega y + Bxy - \gamma_1(z - z_t),
\]

where the local fields are given in Eq. (20). The attenuation parameters \(\gamma_1\) and \(\gamma_2\) can be calculated in the same way as for spin systems \([27]\), being expressed through the particle interactions. In our case, these parameters are of order \(J + B\).

Before solving Eq. (21), it is convenient to reduce them to dimensionless notation. To this end, we define the dimensionless parameters

\[
\omega \equiv \frac{\Omega}{J + B}, \quad b \equiv \frac{B}{J + B},
\]

and notice that \(J/(J + B) = 1 - b\). We also define the dimensionless function of time

\[
h \equiv \frac{D_t}{J + B}.
\]

For the dimensionless damping parameter, we take

\[
\gamma \equiv \frac{\gamma_1}{J + B} = \frac{\gamma_2}{J + B}.
\]

We consider the case of zero temperature and measure time in units of \(1/(J + B)\).

In this way, we come to the system of dimensionless equations describing the tunneling intensity,

\[
\frac{dx}{dt} = (1 - b)yz - \gamma(x - x_t),
\]

Josephson current,

\[
\frac{dy}{dt} = (\omega - x)z - \gamma y,
\]

and the well imbalance,

\[
\frac{dz}{dt} = (bx - \omega)y - \gamma(z - z_t),
\]

with the local fields

\[
x_t = \frac{\omega - bx}{h}, \quad z_t = \frac{(1 - b)z}{h},
\]

where

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

Eq. (25) to Eq. (29) form the main system of evolution equations to be analyzed in what follows. We may notice that these equations are invariant under the change of signs of \(x, y, \) and \(\omega\). Fixing \(\omega\) positive implies that the energy levels in a double well are enumerated so that \(E_1 < E_2\).

### 4. Nonlinear dynamics

First, let us consider the existence and stability of attractors of Eq. (25) to Eq. (27). We keep in mind that, by their definitions,

\[
\omega \geq 0, \quad 0 \leq b < 1.
\]

There are two fixed points that are either stable or unstable depending in the value of \(\omega\).

When the tunneling parameter is in the interval

\[
0 \leq \omega < 1,
\]

the stable fixed point is

\[
x^*_t = \omega, \quad y^*_t = 0, \quad z^*_t = \sqrt{1 - \omega^2}.
\]

The characteristic exponents, defined as the eigenvalues of the Jacobian matrix, will be denoted by \(\lambda\). For the fixed point (32), we have

\[
\lambda_1 = -\gamma \quad (\omega < 1),
\]

and two other exponents are the solutions of the quadratic equation

\[
(1 - b)\lambda^2 + \gamma(2 - b - \omega^2)\lambda + (1 - \omega^2)[(1 - b)^2 + \gamma^2] = 0.
\]

The general solutions of Eq. (34) are easily written, though they are rather cumbersome. For illustration, we represent the characteristic exponents for small \(\gamma < 1\). Then

\[
\lambda_{2,3} = -\frac{(2 - b - \omega^2)}{2(1 - b)}\gamma \pm i \omega_{eff},
\]

with the effective frequency

\[
\omega_{eff} = \sqrt{(1 - b)(1 - \omega^2) \left[1 - \frac{(b - \omega^2)^2\gamma^2}{8(1 - b)^3(1 - \omega^2)}\right]}.
\]

This shows that the fixed point (32), for small \(\gamma\), is a stable focus. The value \(\omega = 1\) is a bifurcation point. When approaching this point, the characteristic exponents \(\lambda_2\) and \(\lambda_3\) are

\[
\lambda_2 \approx \frac{(1 - b)^2 + \gamma^2}{(1 - b)^2} \frac{2(1 - \omega)}{(1 - b)} + \left[\frac{(1 - b)^2 + \gamma^2}{(1 - b)^2} \right] \frac{(1 - \omega)^2}{(1 - b)\gamma^3},
\]

\[
\lambda_3 \approx -\gamma + \frac{2(1 - b)(1 - \omega)}{\gamma} + \left[\frac{4(1 - b)^2 + (3 + b)\gamma^2}{\gamma^3}\right] \frac{(1 - \omega)^2}{\gamma^3},
\]

for \(\omega\rightarrow 1 - 0\). In the limit \(\omega = 1\), the fixed point (32) is neutral, since \(\lambda_2 = 0\). When \(\omega\) grows larger than one, point (32) becomes unstable.
For the tunneling parameter
\[ \omega > 1, \]
the stable fixed point is
\[ x_1^2 = 1, \quad y_1^2 = 0, \quad z_1^2 = 0. \]  
(39)
For the characteristic exponents, we have
\[ \lambda_1 = -\gamma, \quad (\omega > 1) \]  
(40)
and the equation
\[ \lambda^2 + \frac{2\omega - 1 - b}{\omega - b} \gamma + \frac{(\omega - 1)[(\omega - b)^2 + \gamma^2]}{\omega - b} = 0 \]  
(41)
defining \( \lambda_2 \) and \( \lambda_3 \). The latter for small \( \gamma \) are
\[ \lambda_{2,3} \simeq -\frac{2\omega - 1 - b}{2(\omega - b)} \gamma \pm i\omega_{\text{eff}}', \]  
(42)
with the effective frequency
\[ \omega_{\text{eff}}' = \sqrt{(\omega - 1)(\omega - b)} \left[ 1 - \frac{(1 - b)^2\gamma^2}{8(\omega - 1)(\omega - b)^2} \right]. \]  
(43)
Recall that \( b < 1 \), hence \( \omega > b \). When \( \omega \) approaches the bifurcation point from above, that is \( \omega \to 1 + 0 \), then
\[ \lambda_2 \simeq -\frac{(1 - b)^2 + \gamma^2}{(1 - b)\gamma}(\omega - 1) - \frac{[(1 - b)^2 + \gamma^2]^2 - 2\gamma^4(\omega - 1)^2}{(1 - b)^2\gamma^3}, \]  
(44)
\[ \lambda_3 \simeq -\gamma + \frac{1 - b}{\gamma}(\omega - 1) + \frac{(1 - b)^2 + 2\gamma^2(\omega - 1)^2}{\gamma^3}. \]
For \( \omega > 1 \), the fixed point (39) is stable. But at the bifurcation point \( \omega = 1 \), the stationary solution (39) is neutral, since \( \lambda_3 = 0 \). And point (39) becomes unstable for \( \omega < 1 \).

An important observation is that the system of equations (25), (26), and (27) is structurally unstable if \( \gamma = 0 \), since then \( \lambda_1 = 0 \) and \( \lambda_2 \) and \( \lambda_3 \) are purely imaginary. Such a behavior is rather general for the cases not taking into account attenuation [31,32]. Allowance for the damping, due to particle collisions, makes the system structurally stable and substantially influences the overall dynamics. To emphasize the drastic change brought by the inclusion of the attenuation, we solve Eq. (25) to Eq. (27) numerically and present the results in the figures.

Fig. 1 shows the system dynamics for the tunneling parameter in the region (31), when the stable fixed point is given by Eq. (32). The initial conditions correspond to atoms loaded into the lattice in a nonequilibrium state. If the attenuation is not taken into account, the variables oscillate around their initial conditions. But giving due consideration for the attenuation results in the variables relaxing to the related stationary point.

In Fig. 2, the parameters correspond to the stable fixed point (39). Again, at the initial time, atoms are loaded into the lattice in a nonequilibrium state. When there is no damping, all variables oscillate around their initial values. While, the presence of damping forces the variables to relax to their stationary solutions. Varying the parameter \( b \) in the admissible region \( 0 \leq b < 1 \) does not influence much the system dynamics. Changing the tunneling parameter \( \omega \) inside the region (31) also does not yield considerable difference in the system
5. Conclusion

An effective Hamiltonian for ultracold atoms in a double-well lattice is derived. Nonequilibrium situation is considered, when atoms are loaded into the lattice in a state far from a stationary one. As dynamical variables, we analyze the tunneling intensity, Josephson current, and the population displacement. The treatment is done in the local-field approximation, taking into account the attenuation, caused by particle collisions. It is shown that the proper account of damping drastically changes the system dynamics, as compared to the case of no attenuation included. If the simple mean-field approximation, with no damping, is used, the dynamic variables oscillate around their initial values. While taking into consideration the attenuation re-
results in the relaxation of the dynamical variables to their stationary solutions. Depending on the value of the tunneling parameter, there exist two types of stationary solutions, whose main difference is either in the presence of a stationary atomic displacement in a double well, \( z_1^* \neq 0 \), or in its absence, when the atoms in a double well are distributed symmetrically, \( z_2 \neq 0 \).

An important message following from these results is that the so popular simple mean-field approximation should be used with caution. When considering nonlinear dynamics, such a simple approximation, with no account of attenuation, can lead to qualitatively incorrect conclusions.

The results of the present paper are applicable to ultracold particles of different nature. These could be neutral atoms and molecules [7–11] or cold ions [33,34]. The basic requirement that the particles could be loaded into a double-well lattice.

The double-well lattices possess a rich variety of properties, which makes them an attractive candidate for different applications. A very important point is that the lattice properties can be regulated and controlled in a rather wide range. In addition to choosing the appropriate values of the lattice parameters, it is also feasible to realize their temporal modulation, similar to the case of usual optical lattices, whose parameters can be made time dependent by applying external fields [35–37], by moving [3,38], or just by shaking the lattice [39,40].

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