Effective Hamiltonian of an ultracold Bose gas confined in a four-well optical lattice

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In this paper we study an interacting Bose gas at low temperatures, confined in a one-dimensional potential composed of four wells. In order to derive and validate the effective Hamiltonian that describes this system, we study the stationary states of a particle confined in the four-well potential. In particular, we calculate the energies and the corresponding wave functions for the ground state and for the three lowest excited states. It was established that the effective Hamiltonian of a four-well optical lattice is composed of tunneling terms among all the wells, and interaction terms between pairs of particles within the same well.
Keywords: Optical lattices; Bose-Einstein condensation; ultracold interacting.

En este artículo se estudió un gas de Bose con interacciones a bajas temperaturas, confinado en un potencial unidimensional de cuatro pozos. Para deducir y validar el Hamiltoniano efectivo que describe este sistema se estudiaron en detalle los estados estacionarios de una partícula confinada en el potencial de cuatro pozos. En particular, se calcularon las energías y las correspondientes funciones de onda del estado base y los tres primeros estados excitados. Se estableció que el Hamiltonaino efectivo del gas de Bose en una red óptica de cuatro pozos está compuesto de términos de tunelaje entre todos los pozos y términos de interacción entre pares de partículas dentro del mismo pozo.
Descriptores: Redes ópticas; condensación de Bose-Einstein; gases de Bose ultrafrios con interacción.

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1. Introduction

The experimental realization of the Bose-Einstein condensation in 1995, in vapors of rubidium, sodium and potassium vapors [1, 2], has given rise to a new field in the study of these and other ultracold gases: the control and manipulation of highly degenerate neutral atoms [3, 4], that is, systems composed of a large number of particles in the same quantum state. One of the achievements of these degenerate gases are the so called optical lattices in one dimension [5–7]. These are formed when a Bose gas at temperatures close to the condensation temperature is confined in a one dimensional periodic potential composed of a finite number of wells. Such a potential can be produced as a result of the superposition of two counter propagating standing laser beams. Thus, the transport of atoms through the barriers can be controlled experimentally by modifying the optical potential that confines the atoms [8].

The creation of the optical lattices by several experimental groups has motivated the community to study their behavior from a theoretical point of view. A useful tool in the study of these systems is the second quantization formalism. This formalism, supported by the indistinguishable quantum nature of the atoms, is based on the knowledge of a complete set of single-particle wave functions, to establish the Hamiltonian that describes a many-body system [9]. In this context the determination of the energies and their corresponding wave functions of a particle confined in a specific potential results relevant.

The main purpose of the present work is to derive and validate the effective Hamiltonian that describes a gas of bosons confined in an optical lattice composed of four wells. That is, we shall concentrate on a derivation from first principles of the effective Hamiltonian to appropriately describe the many-body system. To obtain this derivation, we study the states of a single particle confined in the four well potential in detail. As we shall see, this analysis justifies the validity of the Hamiltonian and establishes the applicability limits of the Bose-Hubbard (BH) Hamiltonian [10] for a lattice composed of four wells. The BH Hamiltonian has been widely used for describing highly correlated bosonic systems. The main contribution of the present study is to consider the modifications in the BH Hamiltonian when the confining potential is composed of a finite number of wells, particularly an arbitrary potential composed of four wells. The study of the dynamical behavior of the Bose gas inside the finite optical lattice is beyond the scope of this work, and it will be considered in a later study.

Due to the fact that the gases confined in the optical lattices are at very low temperatures, the theoretical study of their dynamics in the second quantization scheme requires only the calculation of the ground state and the first excited states. Therefore, the complete set of single-particle wave functions mentioned above can be safely replaced by a less numerous set. In the particular case of an optical lattice composed of four wells in one dimension, it is enough to know the ground state and the three lowest excited states, if their asso-

ciated energy levels lie below the top of the potential barriers. This is a consequence of the fact that the energy levels of a four-well potential split into sets of four levels, so that the separation among the sets is greater than the separation between the levels in each set [11]. To calculate the first set of energy levels and their corresponding wave functions, in this work we shall use the Split Operator (SO) method, which is applicable to any bounded potential [12]. In this study we concentrate on symmetrical four well potentials in one dimension.

As mentioned before, the optical potential produced by the interference of standing laser beams can be modified with the purpose of controlling the transport of atoms inside the potential. In other words, by varying the depth and width of the potential barriers, the tunneling of the atoms through the barriers can be controlled. Based on the calculation of the wave functions of a single particle in the four well potential, we determined how the effective Hamiltonian that describes the many body system is modified when the potential that confines the atoms is varied.

By using the SO spectral method, we evaluated numerically the energies and the corresponding wave functions associated with the four lowest bound states $\{\varepsilon_n, \varphi_n\}, n = 0, .., 3$ of a particle confined in a four-well potential. To perform such an analysis, we proposed a model potential dependent on 5 parameters. As we shall see, these parameters allow us to consider modifications in the depth and width of the wells.

This work is organized in four sections. In Sec. 2, we derive the effective Hamiltonian that describes an ultracold Bose gas with interactions, confined to the one-dimensional potential composed of four wells. In Sec. 3, we describe briefly the method employed to obtain the energies and the wave functions of a single particle in the potential. Results for the energies and wave functions considering the dependence on the depth and width of the wells are also presented. Finally, in Sec. 4, some conclusions of the present study are given.

2. Effective Hamiltonian of an interacting Bose gas confined in a one dimensional four wells lattice

In the second quantization formalism, the most general Hamiltonian that describes a many body system with interactions between pairs of particles is

$$\mathcal{H} = \int dx \hat{\Psi}^\dagger(x) \left(T(x) + V(x)\right) \hat{\Psi}(x) + \frac{1}{2} \int dx dx' \hat{\Psi}^\dagger(x) \hat{\Psi}^\dagger(x') U(x, x') \hat{\Psi}(x') \hat{\Psi}(x), \quad (1)$$

where $T(x)$ is the kinetic energy operator, $V(x)$ is the external potential that confines the atoms (in this study it is a four-well potential), and $U(x, x')$ is the interaction potential between pairs of particles. The field operators $\hat{\Psi}^\dagger(x)$ and $\hat{\Psi}(x)$ can be written in terms of any complete set of single-particle wave functions as

$$\hat{\Psi}^\dagger(x) = \sum_n \varphi_n^*(x) a_n^\dagger \quad \text{and} \quad \hat{\Psi}(x) = \sum_n \varphi_n(x) a_n, \quad (2)$$

where the operators a_n and $a_n^\dagger$ satisfy the usual commutation rules for bosons $\left[a_n, a_l^\dagger\right] = \delta_{n,l}$. In this work, we model the interactions among the particles through a contact interaction potential

$$U(x, x') = \frac{4\pi\hbar^2 a}{m} \delta(x - x'), \quad (3)$$

where a is the scattering length. We should remark that this model potential is valid in the limit of low energies and in the Born approximation [13]. Due to the fact that in dilute ultracold gases the effect of the interaction among the particles is fully included in the scattering length a, the specific form of the interaction potential does not affect the main qualitative features of the many body description.

The energy levels associated with the bound states of a one-dimensional potential composed of n wells are split into n-tuples of levels such that the separation between the n-tuples is much greater than the separation between the levels in each n-tuple [13]. Therefore, for sufficiently deep wells, the energy spectrum of a particle confined in a potential composed of four wells will be formed by several sets of four levels. Due to the fact that the system under study consists of a Bose gas at very low temperatures, the only relevant states to describe it are the states associated with the lowest energy levels in the four-well potential [11]. Then, for the special case of ultracold bosons, the complete set of single-particle wave functions required in the expressions for the field operators (2) in the second quantization formalism, can be safely replaced by the set $\{\varepsilon_n, \varphi_n\}$, $n = 0, 1, 2, 3$ of the single-particle wave functions in a four-well potential. By adjusting the depths of the potential barriers, one can guarantee that only the first set of energies and its corresponding states is necessary for the description of the Bose gas.

After we substitute the eigenfunctions $\varphi_n(x)$ in Eq. (1), the Hamiltonian $\mathcal{H}$ that describes the many body system becomes

$$\mathcal{H} = \sum_{n=0}^{3} \varepsilon_n a_n^\dagger a_n + \sum_{k,n,l,m=0}^{3} g a_k^\dagger a_n^\dagger a_l a_m, \quad (4)$$

where

$$g = \frac{4\pi\hbar^2 a}{m} \int \varphi_k(x) \varphi_n(x) \varphi_l(x) \varphi_m(x) dx. \quad (5)$$

From this equation we see that the part of the Hamiltonian that involves the kinetic energy and the external potential (that is, the four-well potential) is diagonal, as a consequence of the fact that the field operators (2) were expressed in the basis $\{\varepsilon_n, \varphi_n\}$, $n = 0, 1, 2, 3$. The second term in $\mathcal{H}$ represents the interactions between pairs of particles in different states $\varphi_n(x)$. Thus, the Hamiltonian (4) describes an ultracold gas of bosons with interactions, confined in a potential composed of a finite number of wells in one dimension.

In order to study the dynamics in a finite optical lattice, the Hamiltonian (4) can be rewritten in a more appropriate basis than the extended single particle wave functions $\varphi_n(x)$ [11]. This basis is formed by the localized wave functions in each well, and can be constructed from the extended wave functions $\varphi_n(x)$ as follows:

$$\psi_1(x)=\frac{1}{\sqrt{8}}\left(\varphi_0(x)+\sqrt{3}\varphi_1(x)+\sqrt{3}\varphi_2(x)+\varphi_3(x)\right), \quad (6)$$

$$\psi_2(x)=\frac{1}{\sqrt{8}}\left(\sqrt{3}\varphi_0(x)+\varphi_1(x)-\varphi_2(x)-\sqrt{3}\varphi_3(x)\right), \quad (7)$$

$$\psi_3(x)=\frac{1}{\sqrt{8}}\left(\sqrt{3}\varphi_0(x)-\varphi_1(x)-\varphi_2(x)+\sqrt{3}\varphi_3(x)\right), \quad (8)$$

$$\psi_4(x)=\frac{1}{\sqrt{8}}\left(\varphi_0(x)-\sqrt{3}\varphi_1(x)+\sqrt{3}\varphi_2(x)-\varphi_3(x)\right). \quad (9)$$

This transformation is a generalization of the usual transformation performed in a two-level system when a rotation through 90 degrees is made [13]. For a system of particles confined in an n-well potential, the linear transformation that relates the extended and the localized wave functions is given by the Wigner rotation matrix [14] and has been previously used in Ref. 11. Similarly, the transformation that defines the creation and annihilation operators $b_i^\dagger$ and b_i of particles in each well, in terms of the operators $a_n^\dagger$ and a_n, is the same as the transformation that relates the extended and the localized single-particle wave functions. As we shall see in the next section, the linear combination that defines $\psi_1(x)$ [Eq. (6)] is the probability amplitude of finding a particle localized in well 1; $\psi_2(x)$, ψ_3 y $\psi_4(x)$ are the probability amplitudes of finding a particle localized in the wells 2, 3 and 4, respectively.

Before we write the Hamiltonian $\mathcal{H}$ in the basis of the localized wave functions in each well, we want to emphasize that the energy levels associated with the wave functions $\varphi_n(x)$ do not necessarily need to satisfy the condition of being equally spaced; that is, for a given external potential composed of four wells, those energy levels can satisfy the general relation: $\varepsilon_1-\varepsilon_0=\Delta$, $\varepsilon_2-\varepsilon_1=\Delta/q$, $\varepsilon_3-\varepsilon_2=\Delta/r$, where q y r are two parameters ($q,r>0$) that can be adjusted to specify the separation of the four lowest energy levels in each potential. As we shall see below, when $\mathcal{H}$ is expressed in the basis of the localized wave functions, the transformation of the diagonal term

$$\mathcal{H}_D=\sum_{n=0}^{3}\varepsilon_n a_n^\dagger a_n$$

will be modified as a consequence of the non-equal separation between the lowest energy levels ε_n, $n=0,1,2,3$. The Hamiltonian $\mathcal{H}_D$ becomes in this case:

$$\begin{aligned}\mathcal{H}_D=-\frac{\Delta}{8}\Bigg\{&\sqrt{3}\left(1+\frac{1}{r}+\frac{2}{q}\right)\\ &\times\left[b_1^\dagger b_2+b_2^\dagger b_1+b_3^\dagger b_4+b_4^\dagger b_3\right]\\ &+\left(3+\frac{3}{r}+\frac{2}{q}\right)\left[b_2^\dagger b_3+b_3^\dagger b_2\right]\\ &+\left(1+\frac{1}{r}-\frac{2}{q}\right)\left[b_1^\dagger b_4+b_4^\dagger b_1\right]\\ &+\sqrt{3}\left(1-\frac{1}{r}\right)\left[b_1^\dagger b_3+b_3^\dagger b_1+b_2^\dagger b_4+b_4^\dagger b_2\right]\Bigg\}. \quad (10)\end{aligned}$$

From this expression for $\mathcal{H}_D$, we see that the tunneling terms between non-adjacent wells become zero when parameters q and r are equal to 1, that is, when the energy levels are equally spaced. In other words, the effective Hamiltonian that describes a Bose gas with no interactions, confined in an arbitrary four well potential $V(x)$, will be composed of tunneling terms between all the wells unless such a potential possesses equally-spaced energy levels.

After we substitute the localized wave functions and their corresponding creation and annihilation operators in the second term of Hamiltonian $\mathcal{H}$, that is, in the interaction term

$$\mathcal{H}_I=\sum_{k,n,l,m=0}^{3} g a_k^\dagger a_n^\dagger a_l a_m,$$

we find the interaction of particles in different wells. However, if the overlap between the localized wave functions $\psi_i(x)$ can be neglected, the integral of any arbitrary product of four localized wave functions

$$\int \psi_i(x)\psi_j(x)\psi_k(x)\psi_l(x)dx$$

can be considered to be equal to zero. Thus, the Hamiltonian that describes the interaction term of the Hamiltonian $\mathcal{H}$ will be:

$$\mathcal{H}_I=\frac{4\pi\hbar^2 a}{m}\sum_{i=1}^{4} b_i^\dagger b_i^\dagger b_i b_i, \quad (11)$$

that is, it contains only interactions of particles within the same well. Considering both contributions $\mathcal{H}_D$ and $\mathcal{H}_I$, the Hamiltonian that describes bosons with interactions in a four well potential $V(x)$ whose energy levels are equally spaced is:

$$\begin{aligned}\mathcal{H}=-\Delta\Bigg\{&\frac{\sqrt{3}}{2}\left[b_1^\dagger b_2+b_2^\dagger b_1+b_3^\dagger b_4+b_4^\dagger b_3\right]\\ &+\left[b_2^\dagger b_3+b_3^\dagger b_2\right]\Bigg\}+\frac{4\pi\hbar^2 a}{m}\sum_{i=1}^{4} b_i^\dagger b_i^\dagger b_i b_i. \quad (12)\end{aligned}$$

From this Hamiltonian we can conclude that the dynamics of a Bose gas confined in a four well potential will be described by the coefficients Δ and a, that is, the tunneling

coupling coefficient between adjacent wells, and the coefficient a that modulates the interaction between pairs of particles within the same well.

In the next section we shall study in detail the wave functions of a particle confined in a one-dimensional potential composed of four wells, in particular, the eigenfunctions associated with the lowest bound states. Such an analysis will allow us to validate the effective Hamiltonian 12, and to establish the conditions under which the Bose-Hubbard Hamiltonian correctly describesan optical lattice composed of four wells. This Hamiltonian has been widely used in describing finite optical lattices in one dimension. As is well known, the Bose-Hubbard Hamiltonian establishes that particles can tunnel only between adjacent wells with equal probability, and interactions among the particles occur within the same well. The main purpose of the present work is to establish how this Hamiltonian is modified for a finite potential, in particular for a potential composed of four wells.

3. Wave functions of a particle in a one-dimensional four well potential

In this section we determine the energies and the wave functions of a particle with mass m described by the Hamiltonian

$$H = \frac{p^2}{2m} + V(x), \tag{13}$$

where the functional form of $V(x)$ is

$$V(x) = V_1 x^{10} + A_1 e^{-\frac{(x+a)^2}{2\sigma_1^2}} + A_2 e^{-\frac{x^2}{2\sigma_2^2}} + A_1 e^{-\frac{(x-a)^2}{2\sigma_1^2}}. \tag{14}$$

In this equation, parameters A_i and σ_i take into account the possibility of varying the depth and the width of the wells, while the coefficient V_1 is used to ensure that the particle moves inside the four-well potential. The center of each well can be modified through parameter a.

By using the Split Operator (SO) method introduced by M.D. Feit and J.A. Fleck [12] we determine the four lowest energy levels and their corresponding wave functions, associated with the bound states of a particle confined in the potential $V(x)$. The energies and wave functions of those levels will be denoted as $(\varepsilon_n, \varphi_n)$, $n = 0, 1, 2, 3$.

The SO method is based on the spectral decomposition of an initial wave function $\psi(x, 0)$ in terms of the eigenfunctions of the Hamiltonian (13):

$$\psi(x, 0) = \sum_n c_n \varphi_n(x). \tag{15}$$

This decomposition can be obtained from the temporal evolution of the initial wave function as described below.

In the temporal evolution operator

$$U(t) = \exp\left[\frac{-iHt}{\hbar}\right], \tag{16}$$

the kinetic energy operator $\hat{p}^2/2m$, must be divided into two equal parts, such that the temporal evolution of the initial state $\psi(x, 0)$ after an interval Δt is given by:

$$\psi(x, \Delta t) \approx e^{-i\frac{\hat{p}^2}{2m}\frac{\Delta t}{2\hbar}}\, e^{-iV(x)\frac{\Delta t}{\hbar}}\, e^{-i\frac{\hat{p}^2}{2m}\frac{\Delta t}{2\hbar}} \psi(x, 0). \tag{17}$$

Due to the non-commutation of the operators $\hat{p} = -i\hbar d/dx$ and $V(x)$, this equation is valid up to the second order, that is, the first errors do not appear until the third order in Δt. The successive application of the temporal evolution to the initial state $\psi(x, 0)$ in intervals Δt allows us to obtain the state at a posterior time t.

The initial wave function $\psi(x, 0)$ can be chosen in an almost arbitrary way. However, in order to obtain an energy spectrum with even and odd values, this function must not have a definite parity. For the present analysis, we shall use as the initial wave function a gaussian function centered in the first well.

In order to obtain the energies and their corresponding wave functions, it is necessary to define the correlation function between the initial state and the state at time t as:

$$\mathcal{P}_1(t) = \langle \psi(0) | \psi(t) \rangle. \tag{18}$$

By expressing the function $\psi(x, t)$ as a linear superposition of the eigenfunctions of H,

$$\psi(x, t) = \sum_n c_n \varphi_n(x) e^{-i\varepsilon_n t/\hbar}, \tag{19}$$

the correlation function $\mathcal{P}_1(t)$ can be rewritten as

$$\mathcal{P}_1(t) = \sum_n |c_n|^2 e^{-i\varepsilon_n t/\hbar}, \tag{20}$$

whose Fourier transform is

$$\mathcal{P}_1(\varepsilon) = \sum_n |c_n|^2 \delta(\varepsilon - \varepsilon_n). \tag{21}$$

From this equation one can read directly the energy eigenvalues ε_n for a given potential $V(x)$.

It is important to note that, in the above lines, the knowledge of $\mathcal{P}_1(t)$is implicit for all times. In order to take into account the finite size of our sampling ($0 < t < T$), is necessary the introduction of a special function $w(t)$, called the normalized Hanning window function [12]. By multiplying the correlation $\mathcal{P}_1(t)$ by $w(t)/T$, we obtain, in the reciprocal space, the energy spectrum identifying the "peaks" associated with different values of ε_n for a given potential $V(x)$.

The wave functions associated with the eigenvalues ε_n can also be determined from the spectral decomposition method. To do so, we must perform a numerical integration as follows:

$$\varphi_n(x) = N \int_0^T \psi(x, t) w(t) \exp(i\varepsilon_n t) dt = N\psi(x, \varepsilon_n).$$

For the potential model (14), we considered 22 different sets of parameters $\{A_i, V_i, \sigma_i, a\}$ to determine the four lowest energy levels. For purposes of, illustration, we selected three of these sets to show the dependence of the eigenenergies on the choice of the parameters. From our analysis, we want to remark first that the separation between these energy levels is highly dependent on small changes of the parameters. As stated above, we illustrate the results obtained for the 3 different sets of parameters. We shall denote these potentials as $V_1(x)$, $V_2(x)$ y $V_3(x)$.

In Table I, the parameters associated with each potential are specified. The eigenvalues of the energy for the ground state and the three lowest excited states are shown in Table II. In Fig. 1 we plot the potentials $V_1(x)$, $V_2(x)$ y $V_3(x)$; the horizontal lines in each case indicate the energy levels. As can be observed, all of these levels correspond to bound states inside the four well potential. From this figure, one can also observe that the energy levels satisfy the following conditions:

i) for $V_1(x)$, $\varepsilon_2 - \varepsilon_1 < \varepsilon_1 - \varepsilon_0 = \varepsilon_3 - \varepsilon_2$,

ii) for $V_2(x)$, $\varepsilon_3 - \varepsilon_2 \approx \varepsilon_2 - \varepsilon_1 \approx \varepsilon_1 - \varepsilon_0$, and

iii) for $V_3(x)$, $\varepsilon_2 - \varepsilon_1 > \varepsilon_1 - \varepsilon_0 = \varepsilon_3 - \varepsilon_2$.

We should point out that it is essential that the potential barriers in each case should be deep enough in order to guarantee that at least four bound states exist in each potential. This assumption is necessary to justify the use of the basis $\{\varphi_n(x),\ n = 0, ..3\}$ in the many body Hamiltonian (1).

In Fig. 1a we illustrate the energy for the case in which the wells in the center have approximately half of the width of the wells in the exterior. By using the notation introduced in the previous section for the separation between levels, we get $q \approx 2.91$ and $r \approx 1.04$. From our analysis, we observe that, as the width of the central wells is reduced with respect to the exterior wells, the levels ε_1 and ε_2 tend to the same value, while the levels ε_0 and ε_3 separate from ε_1 and ε_2 in the same proportion.

TABLE I. The values of the parameters listed in this table determine in each case the specific potential of Eq. (2).

Potential	V_1	A_1	A_2	σ_1	σ_2	a
$V_1(x)$	4.0×10^{-7}	8.10	6.50	1.118	0.500	2.500
$V_2(x)$	1.9×10^{-7}	4.40	3.30	0.576	0.650	2.625
$V_3(x)$	2.7×10^{-7}	4.30	3.70	0.420	0.700	2.625

TABLE II. Eigenvalues of the energy associated with the four lowest bound states of the potentials $V_1(x)$, $V_2(x)$ y $V_3(x)$.

Potential	ε_0	ε_1	ε_2	ε_3
$V_1(x)$	0.7032	0.8846	0.9468	1.1208
$V_2(x)$	0.5672	0.7002	0.8184	0.9483
$V_3(x)$	0.6039	0.7116	0.8957	1.0057

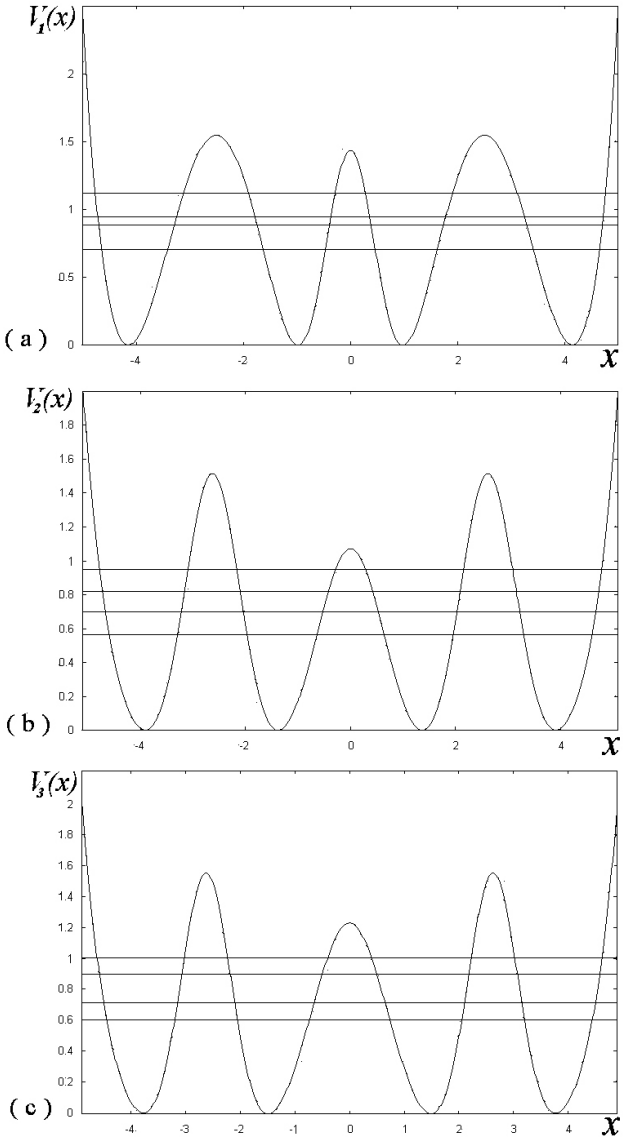

FIGURE 1. The potentials analyzed with the Split Operator SO method are shown, Figs. (a), (b) and (c) correspond to the potentials $V_1(x)$, $V_2(x)$ y $V_3(x)$ of Table I respectively. In each potential, the horizontal lines indicate the four lowest energy levels ε_0, ε_1, ε_2, y ε_3.

In Fig. 1b, we show the results for $V_2(x)$. In this case we chose the parameters σ_i and V_i such that the consecutive energy levels have almost the same spacing, *i.e.* we get $q \approx r \approx 1.0$. In comparison with the results obtained for potential $V_1(x)$, we observe that this condition requires that the widths of the four wells become almost equal, and that the exterior wells be deeper than the central wells.

For the potential $V_3(x)$ (Fig. 1c), the parameters are chosen such that the energy levels have opposite characteristics than those obtained for the potential $V_1(x)$. In order to observe this effect, we need only vary the width of the wells. In this case we found $q \approx 0.58$ and $r \approx 0.97$.

The wave functions in arbitrary units associated with the set of energies $\{\varepsilon_n, n = 0, 1, 2, 3\}$ for each potential, are

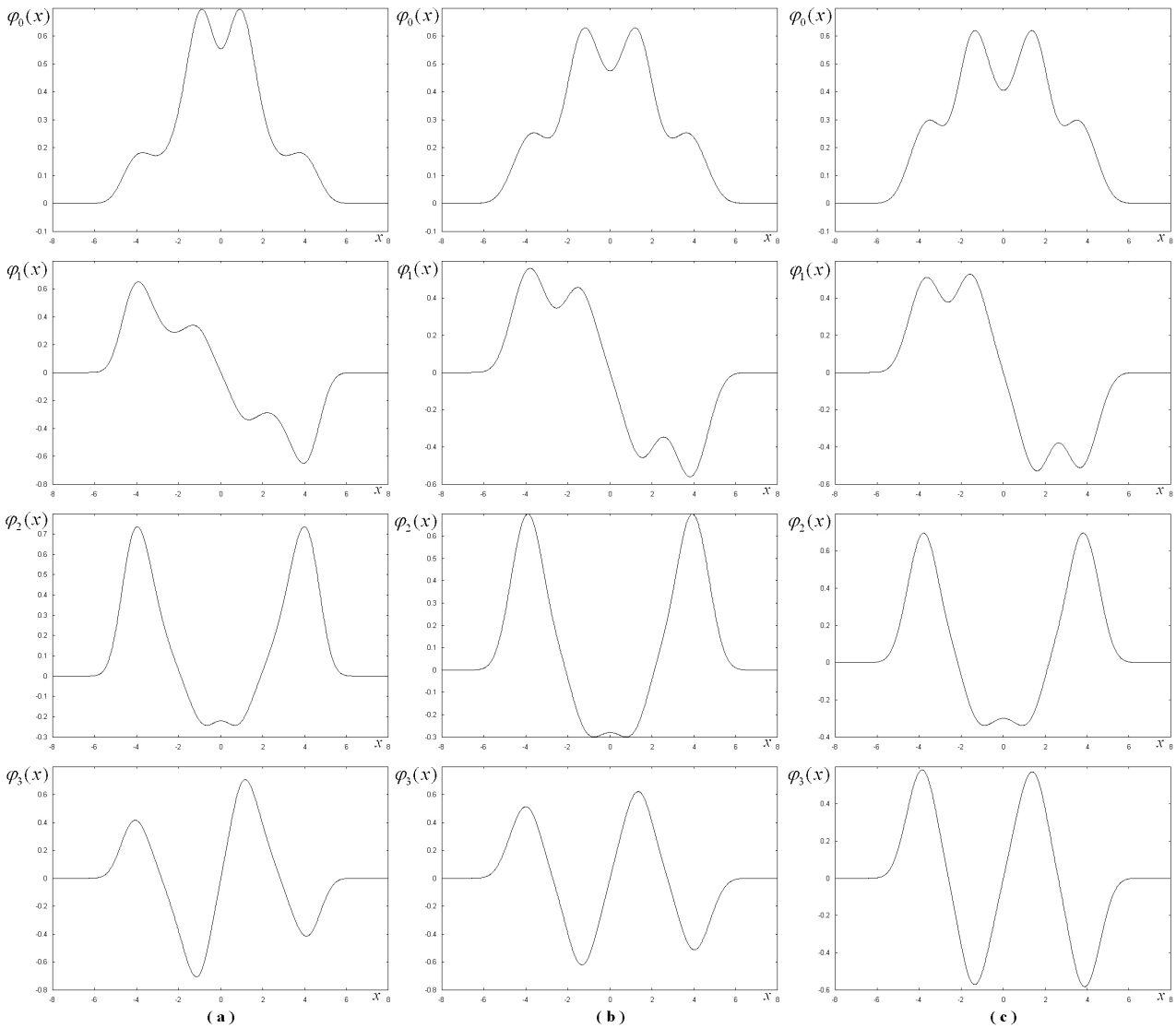

FIGURE 2. Figures (a), (b), and (c) show the wave functions in arbitrary units associated with the energy levels ε_0, ε_1, ε_2, y ε_3, of a particle confined in the potentials $V_1(x)$, $V_2(x)$ and $V_3(x)$, respectively.

shown in Fig. 2. The Figs. 2a, 2b and 2c correspond to potentials $V_1(x)$, $V_2(x)$, y $V_3(x)$ respectively.

From this analysis, we observe that while the values of the energy have high sensitivity to the choice of parameters $\{A_i,\ V_i,\ \sigma_i, a\}$, the associated wave function, as expected, has the same structure. We found numerically that the overlap between the extended wave functions in the same state is at least 95%.

In the light of Eq. (10), we see that if the energy levels of a given potential $V(x)$ are not equally spaced, *i.e.* if the parameters q and r are different from 1, then in the effective Hamiltonian (12) tunneling terms between non-adjacent wells must be considered. In a previous study for the dynamics of a Bose gas confined in a three-well potential [15], it was demonstrated that the dynamics is substantially modified when tunneling terms between non-adjacent wells are included.

From the extended wave functions $\varphi_n(x)$, the localized wave functions in each well $\psi_i(x)$ can be constructed using the Eqs. (6)-(9). In Fig. 3, these localized wave functions in arbitrary units for the potential $V_2(x)$ are shown. From this figure, we observe that the overlap between any of these functions $\psi_i(x)$ and $\psi_j(x)$ can be considered to be negligible. We numerically verified that this overlap is smaller than 1% in each case. Thus, according to what was established in the previous section

$$\text{(if} \quad \int \psi_i(x)\psi_j(x)dx \approx \delta_{i,j}$$

$$\text{then} \quad \int \psi_i(x)\psi_j(x)\psi_k(x)\psi_l(x)dx \approx 0),$$

it is well justified that the effective Hamiltonian $\mathcal{H}_I$ have interactions only between particles within the same well.

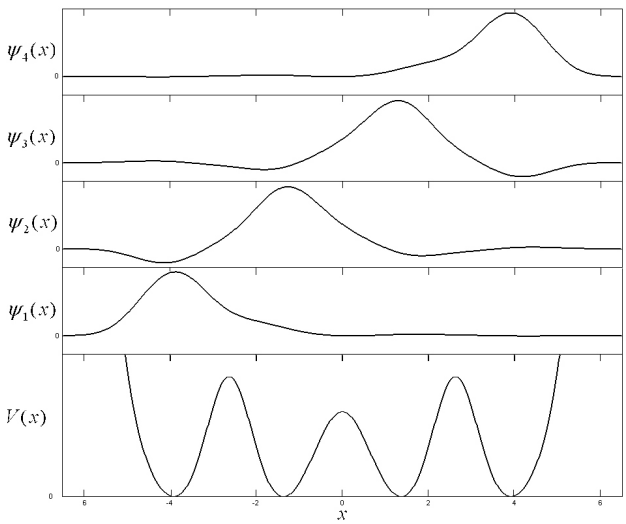

FIGURE 3. The localized wave functions in arbitrary units of a particle in the potential $V_2(x)$ are shown (see Fig. 1).

We can conclude that if the confining four-well potential is such that the tunneling coupling coefficients are not negligible, the dynamics in an optical lattice of four wells using the Bose-Hubbard Hamiltonian is not fully accurate. However, it is well justified that in this Hamiltonian only interactions between particles in the same well be taken into account.

4. Conclusions

In this work, we have derived and validated the effective Hamiltonian that describes a Bose gas with interactions, at very low temperatures, when it is confined in a potential in one dimension composed of four wells. That is, from first principles we performed a derivation of the effective Hamiltonian that represents the many-body system. In order to validate this Hamiltonian, we studied in detail the energies and the wave functions of a single particle confined in such a potential ($\{\varepsilon_n, \varphi_n(x)\}$). In particular, we obtained the wave functions associated with the lowest bound states. By using a linear transformation, the localized wave functions in each well $\psi_i(x)$ were constructed in terms of the extended wave functions $\varphi_n(x)$.

We used as an assumption the fact that, in an ultracold Bose gas, only the lowest states are occupied. Then, working in the second quantization formalism, we considered as a complete basis the set $\{\varphi_n(x),\ n = 0, ..3\}$, to derive the effective Hamiltonian that describes the system of bosons with interactions. In the basis of the localized wave functions in each well, we found that this Hamiltonian is composed of terms describing the tunneling between all the wells, and interaction terms between particles within the same well.

Based on the study of the stationary wave functions, that is, the extended wave functions, we demonstrated that, if the four lowest energy levels in the potential are equally spaced, only tunneling terms between adjacent wells become relevant in the description of the many body system. From our analysis, we also concluded that the fact that only interactions between particles in the same well appear in the effective Hamiltonian is a consequence of assuming that the overlap between the localized wave functions can be neglected.

Transport of ultracold Bose gases confined in potentials composed of three wells has been studied in previous works [11,15]. In those studies it was observed that the dynamics of the particles is governed by the tunneling energy Δ and the coefficient that modulates the interaction g. Although the tunneling dynamics in a four-well potential is beyond the scope of this work, we can safely extrapolate that the temporal evolution of this system will have qualitative features similar to those observed for the three-well system.

It is important to note that the dynamics of an arbitrary optical lattice composed of four wells will be described by an effective Hamiltonian that contains tunneling terms among all the wells. In other words, the experimental realization of an optical lattice in which the particles can tunnel only between adjacent wells requires a precise tuning of the optical potential creating it.

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