Analytical results for energy spectrum and eigenstates of a Bose-Einstein condensate in a Mott insulator state

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We present a method to solve the model describing either a Bose-Einstein condensate (BEC) in a Mott-insulator state or a double-well BEC. We show that all the energy eigenvalues and eigenstates for an *arbitrary* (small or large) total atom number N can be explicitly expressed analytically in terms of a parameter λ whose values are determined by the roots of the polynomials of the order of at most $1+\mathrm{int}(N/2)$, with $\mathrm{int}(x)$ denoting x's integer part. We also show that λ's explicit analytical expressions for $N\leqslant 7$ can be readily obtained by a simple MATHEMATICA code. Besides, finding the roots of the polynomials of the order of at most $1+\mathrm{int}(N/2)$ to give explicitly all the energy eigenvalues and eigenstates greatly simplifies the corresponding calculations, particularly when the total atom number N is large.

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I. INTRODUCTION

Recently, the superfluid–Mott-insulator phase transition has been observed in a system of Bose condensed atoms immersed in a periodic array of optical potentials [1]. In the experiment, the average occupations per well (site) was around one to three atoms, which could potentially form elementary building blocks for atomic qubit based quantum computing designs [2]. Most recently, a scheme has been proposed to create massive maximum entangled pairs, triplets, quartiles, and other clusters of Bose condensed atoms in a Mott-insulator state [3]. In a Mott state, the system dynamics is rather simple as there exists a fixed (small) number of atoms within each well. If we use the second-quantized operators $a(a^\dagger)$ and $b(b^\dagger)$ for atoms in the two internal states, the effective Hamiltonian can be expressed as [3,4]

$$H=2gJ_z^2+2\Omega J_y. \tag{1}$$

The second term denotes the single-atom Raman coupling due to external laser fields with a (real) effective Rabi frequency 2Ω. The angular-momentum operators are the Schwinger representation in terms of the two boson modes,

$$J_x=\frac{1}{2}(b^\dagger a+a^\dagger b),$$

$$J_y=-\frac{i}{2}(b^\dagger a-a^\dagger b), \tag{2}$$

$$J_z=\frac{1}{2}(b^\dagger b-a^\dagger a),$$

with the conserved squared angular momentum $J^2=\Sigma_{k=x,y,z}J_k^2=(N/2)[(N/2)+1]$. The Hamiltonian (1) can also describe a double-well Bose-Einstein condensate with $a(a^\dagger)$ and $b(b^\dagger)$ for condensed atoms in the left and right wells, respectively. To see this point more clearly, we introduce two bosonic annihilation operators $a_1\equiv -ia$ and $a_2\equiv b$ equally denoting condensed atoms in the left and right wells, respectively, and then the Hamiltonian can be, after omitting an unimportant constant $-gN^2/2$ ($N=a^\dagger a+b^\dagger b\equiv a_1^\dagger a_1+a_2^\dagger a_2$ denotes the total number of atoms in the systems and is a conserved quantity), expressed in another form

$$H=\Omega(a_1^\dagger a_2+a_2^\dagger a_1)+g[(a_1^\dagger)^2a_1^2+(a_2^\dagger)^2a_2^2], \tag{3}$$

which is exactly the model utilized to describe a double-well Bose-Einstein condensate [5–9].

Although model (1) or (3) has important applications to the fields of Bose-Einstein condensates, quantum computation and information, no one seems to have been able to solve for the combined dynamics analytically even for a small number of atoms for such system [3,5–7], and it becomes increasingly more painful to obtain analytical results when the total atom number is large. The mean-field method [5–10], number-conserving Bogoliubov theory [11,12], and numerical computations are usually utilized to solve such kind of models. Another powerful method to deal with such models is to utilize the properties of the group or Lie algebra for the Schwinger representation and generalized Schwinger presentations [13,14]. Progress has been achieved towards understanding the characteristics of the spectrum and eigenstates for models (1) and (3) [13]. In view of its importance, it is thus desirable to develop a simple and efficient method to obtain analytically the energy spectrum and eigenstates for model (1) or (3) at least for a small number of atoms.

In this paper, we shall present an efficient and simple method to solve model (1) or (3) based on the approach proposed by us [15]. We show that all the energy eigenvalues and eigenstates for an *arbitrary* (small or huge) total atom number N can be explicitly expressed analytically in terms of a parameter λ while its values are determined by the roots of a polynomial of the order of at most $1+\mathrm{int}(N/2)$. We show that we can obtain λ's explicit analytical expressions for $N\leqslant 7$, and hence give all the energy eigenvalues and eigen-

states in terms of the given parameters Ω and g of Eq. (3), which should be helpful for preparation, manipulation and control of a Bose-Einstein condensate in optical lattices in a Mott-insulator state or of a double-well Bose-Einstein condensate, and for facilitating the investigation of massive maximum entangled pairs, triplets, quartiles, and other clusters of Bose condensed atoms in such systems. Besides, finding the roots of the polynomials of the order of at most $1+\mathrm{int}(N/2)$ to give explicitly all the energy eigenvalues and eigenstates greatly simplifies the corresponding numerical calculations, particularly when the total atom number N is large.

The paper is organized as follows. In Sec. II, we describe the simple method to reduce the corresponding eigenvalue problem into a differential equation. In Sec. III, we first discuss how to simplify the method, and then we present the analytical expressions of all the energy eigenvalues and eigenstates in terms of a parameter λ which can be obtained by finding the roots of the polynomials of the order of at most $1+\mathrm{int}(N/2)$. In Sec. IV, we list explicitly the analytical expressions of the parameter λ for small N. In Sec. V, we discuss the results in some limiting cases. Section VI concludes the paper with a summary.

II. PROCEDURE FOR THE EIGENVALUE EQUATION

In this section, we describe how to reduce the corresponding eigenvalue problem into a differential equation by the method proposed by us [15]. We shall focus on model (3) but all the final results are equally suitable for model (1) except for different eigenvalues E [adding a constant $-gN^2/2$ to the eigenvalues E of model (3) results in those of the model (1)].

The eigenvalue equation for the Hamiltonian (3),

$$H|\Psi_{E,N}\rangle = E|\Psi_{E,N}\rangle, \tag{4}$$

can be reduced into an operator-type differential equation by the following steps [15]. Let us denote the energy eigenstates as

$$|\Psi_{E,N}\rangle = F(a_1^\dagger, a_2^\dagger)|\mathrm{vac}\rangle, \tag{5}$$

where F is a polynomial of the creation operators $a_{1,2}^\dagger$, and the vacuum state $|\mathrm{vac}\rangle = |n_1=0, n_2=0\rangle$ denotes a Fock state without any bosons. Throughout this paper, states $|n_1,n_2\rangle$ denote Fock states with n_j in the jth mode so that $|n_1,n_2\rangle = (1/\sqrt{n_1!n_2!})a_1^{\dagger n_1}a_2^{\dagger n_2}|\mathrm{vac}\rangle$. Then noting $HF|\mathrm{vac}\rangle = ([H,F]+FH)|\mathrm{vac}\rangle = [H,F]|\mathrm{vac}\rangle$ because of the fact $H|\mathrm{vac}\rangle = 0$ due to $a_j|\mathrm{vac}\rangle = 0$, it is seen that the eigenvalue equation becomes $([H,F]-EF)|\mathrm{vac}\rangle = 0$. Finally, by using the identities $a_j|\mathrm{vac}\rangle = 0$, $[a_j^\dagger, F] = 0$, $[a_j^2, F] = a_j[a_j,F] + [a_j,F]a_j = [a_j,[a_j,F]] + 2[a_j,F]a_j$, and $[a_j,F] = \partial F/\partial a_j^\dagger$ (and hence $[a_j,[a_j,F]] = \partial^2 F/\partial a_j^{\dagger 2}$), it is then straightforward to show that the polynomial F of the creation operators $a_{1,2}^\dagger$ satisfies the operator-type differential equation as follows:

$$\Omega\left(x_1\frac{\partial F}{\partial x_2} + x_2\frac{\partial F}{\partial x_1}\right) + g\left(x_1^2\frac{\partial^2 F}{\partial x_1^2} + x_2^2\frac{\partial^2 F}{\partial x_2^2}\right) = EF, \tag{6}$$

where $x_{1,2} \equiv a_{1,2}^\dagger$, F is a polynomial of the form $F(x_1,x_2) = \sum_{j=0}^N \alpha_j x_1^j x_2^{N-j}$ or energy eigenstates $|\Psi_{E,N}\rangle = F(a_1^\dagger, a_2^\dagger)|\mathrm{vac}\rangle \equiv \sum_{j=0}^N c_j|j,N-j\rangle$ with $c_j = \sqrt{j!(N-j)!}\,\alpha_j$.

It is important to note that the operator-type differential equation (6) can formally be thought of as a c-number differential equation because all the operators involved in it are mutually commutable with each other and hence can be solved by any ordinary techniques and/or computer programs for a c-number differential equation [15]. Therefore, we shall hereafter consider Eq. (6) as a c-number differential equation for a c-number polynomial $F(x_1,x_2)$ of the form

$$F(x_1,x_2) = \sum_{j=0}^N \alpha_j x_1^j x_2^{N-j} \equiv x_2^N f(z), \quad z = x_1/x_2. \tag{7}$$

Equations (6) and (7) lead to the differential equation for $f(z) = \sum_{j=0}^N \alpha_j z^j$ as follows:

$$2\tilde{g}z^2\frac{d^2 f(z)}{dz^2} + [1 - z^2 - 2(N-1)\tilde{g}z]\frac{df(z)}{dz} + (Nz-\lambda)f(z) = 0, \tag{8}$$

where $\tilde{g} = g/\Omega$ and the parameter λ relates to the energy eigenvalues by the relation

$$E = gN(N-1) + \Omega\lambda, \tag{9a}$$

$$|\Psi_{\lambda,N}\rangle \equiv |\Psi_{E,N}\rangle = \sum_{j=0}^N \alpha_j\sqrt{j!(N-j)!}\,|j,N-j\rangle. \tag{9b}$$

The unknown parameter λ and coefficients α_j in the polynomial $f(z)$ are determined by solving Eq. (8), and they can also be obtained by solving the matrix equation

$$A\alpha = \lambda\alpha, \tag{10}$$

where A is a $(N+1)\times(N+1)$ tridiagonal matrix with the matrix elements $A_{j,k} = a(j)\delta_{j,k} + (j+1)\delta_{j+1,k} + (N-k)\delta_{j,k+1}$ $(j,k=0,1,\ldots,N)$, $a(j) = 2\tilde{g}j(j-N)$, and $\alpha = (\alpha_0,\alpha_1,\ldots,\alpha_N)^T$ is a column vector with $(N+1)$ components. Equation (10) is obtained simply by substituting $f(z) = \sum_{j=0}^N \alpha_j z^j$ into Eq. (8).

We have now reduced solving the energy eigenvalue equation (4) with the Hamiltonian (3) into finding all the possible λ's values and the corresponding coefficients α_j through solving Eq. (8) or (10). An interesting feature is that if eigenvalue $\lambda(\tilde{g})$ (i.e., λ as a function of $\tilde{g}$) and polynomial $f(z) = \sum_{j=0}^N \alpha_j z^j$ represent a solution to Eq. (8), then $-\lambda(-\tilde{g})$ and the polynomial $f(z) = \sum_{j=0}^N (-1)^j \alpha_j z^j$ must also be a solution. This feature is revealed in a similar model [10] and originates from the fact that Eq. (8) is invariant under the transformation $(\tilde{g},z,\lambda) \to -(\tilde{g},z,\lambda)$. Before end-

ing this section, it is pointed out that the states in Eq. (9b) are also eigenstates for model (1) with the corresponding energy eigenvalues $E=gN(N-1)-gN^2/2+\Omega\lambda=gN(N-2)/2+\Omega\lambda$.

III. ANALYTICAL EXPRESSIONS OF THE ENERGY EIGENVALUES AND EIGENSTATES

We now show that the procedure determining all the possible λ's values and the corresponding coefficients α_j by Eq. (10) can be simplified greatly, and that the analytical expressions of all the energy eigenstates can be obtained explicitly in terms of the parameter λ while λ's values can be obtained by finding the roots of the polynomials of the order of at most $1+\mathrm{int}(N/2)$.

Defining an ''antidiagonal'' $(N+1)\times(N+1)$ matrix S with matrix elements $S_{ij}=\delta_{i,N-j}$ $(i,j=0,1,2,\ldots,N)$, it is straightforward to see that $S\equiv S^{-1}$ with its eigenvalues $s=\pm 1$. What is more important, it is readily shown that it commutes with the matrix A in Eq. (10), i.e., $SA=AS$ and hence $AV_s\subseteq V_s$. Here V_s denotes the subspace spanned by the eigenvectors of the matrix S with eigenvalue s. Consequently, we can choose column vectors $\alpha=(\alpha_0,\alpha_1,\ldots,\alpha_N)^T$ in Eq. (10) to be simultaneously the eigenvectors of the two matrices A and S, implying that the components of all the A's eigenvectors $\alpha=(\alpha_0,\alpha_1,\ldots,\alpha_N)^T$ in Eq. (10) can be chosen to satisfy $S\alpha=s\alpha$ or the relations $\alpha_j=s\alpha_{N-j}$ for $j=0,1,2,\ldots,N$ with $s=\pm 1$. This feature can also be expressed as

$$(\alpha_0,\alpha_1,\ldots,\alpha_N)^T\equiv(s\alpha_N,s\alpha_{N-1},\ldots,s\alpha_0)^T, \quad (11)$$

with $s=\pm$.

Substituting Eq. (11) into Eq. (10), and after some manipulation, it is shown in the Appendix that we can obtain the analytical expressions of all the energy eigenvalues and eigenstates in terms of the parameter λ which is determined by the roots of the polynomials of the order of at most $1+\mathrm{int}(N/2)$. We list the final results here. All the eigenvalues and eigenstates for the Hamiltonian (3) have the forms

$$E=gN(N-1)+\Omega\lambda, \quad (12a)$$

$$|\Psi_{\lambda,N}\rangle=\sum_{j=0}^{\mathrm{int}(N/2)}\frac{C}{1+\delta_{j,N/2}}\sqrt{\frac{(N-j)!}{N!j!}}\det W^{(j)}(\lambda)(|j,N-j\rangle+s|N-j,j\rangle), \quad (12b)$$

where $s=\pm$, $\mathrm{int}(x)$ denotes the x's integer part, and the parameter λ is determined by

$$\det W^{(s)}(\lambda)=0, \quad s=\pm, \quad (13)$$

with $W^{(s)}(\lambda)$ denoting two $(q^{(s)}+1)\times(q^{(s)}+1)$ trigonal matrices of the matrix elements

$$W_{ij}^{(s)}(\lambda)=a_j^{(s)}(\lambda)\delta_{i,j}-\delta_{i+1,j}-p_{i-1}^{(s)}\delta_{i,j+1}, \quad (14)$$

where $i,j=0,1,\ldots,q^{(s)}$, $q^{(s)}=\mathrm{int}(N/2)-\delta_{s,-}\delta_{j,N/2}$, $a_j^{(s)}(\lambda)=\lambda-2\tilde{g}j(j-N)-s(N+1)\delta_{j,(N-1)/2}/2$, and $p_j^{(s)}=(j+1)[(N-j)+\delta_{s,+}\delta_{j+1,N/2}(N/2+1)]$. In Eq. (12b), $\det W^{(0)}(\lambda)\equiv 1$ and $W^{(j)}(\lambda)$ [for $j=1,2,\ldots,\mathrm{int}(N/2)$] is a $j\times j$ trigonal matrix made of the first j rows and columns of the matrix $W^{(s)}(\lambda)$, i.e., $W^{(0)}(\lambda)\equiv 1$ and $W_{i,k}^{(j)}(\lambda)=[\lambda-2\tilde{g}i(i-N)]\delta_{i,k}-\delta_{i+1,k}-i(N+1-i)\delta_{i,k+1}$ $[i,k=0,1,\ldots,(j-1)]$ for $j\leqslant 0$. It is pointed out that $\det W^{(N/2)}=0$ in Eq. (12b) for $s=-$ in the even N case because it is identical to $\det W^{(-)}(\lambda)$ in Eq. (13).

Equations (12) and (13) are the central results of the present paper. Equation (12b) explicitly gives the analytical expressions of all the energy eigenstates for arbitrary positive integers N in terms of the parameter λ. Once λ's values are obtained by solving Eq. (13), all the energy eigenvalues and eigenstates are then explicitly given by Eq. (12). It is pointed out that solving the eigenvalue problem of an $N\times N$ matrix in Eq. (10) have been reduced into just finding the roots of the polynomials of the order of at most $1+\mathrm{int}(N/2)$ [$\det W^{(s)}(\lambda)$ in Eq. (13) leads to the polynomial of the order of $1+q^{(s)}=1+\mathrm{int}(N/2)-\delta_{s,-}\delta_{j,N/2}\leqslant 1+\mathrm{int}(N/2)$ for the parameter λ], which represents a great simplification, particularly when the total atom number N is large.

The explicit analytical expressions of the determinants $\det W^{(k)}(\lambda)$ $k=1,2,\ldots$ (and hence the eigenstates), given by Eq. (12b) for an arbitrary but fixed positive integer N can be easily calculated by a simple MATHEMATICA code *p[j_]:=(j+1)(n-j); a[j_]:=λ-2gj(j-n); n=designated integer; k=designated integer; s=1 or −1; q=Table [a[i−1] Kronecker Delta[i,j] −Kronecker Delta[i+1,j]−p[i−2]Kronecker Delta[i,j+1], {i,k}, {j,k}]; Matrix Form[q]; Det[q]*. Here we list the explicit analytical expressions of the eigenstates given by Eq. (12b) for $N\leqslant 7$ as follows (the overall normalization constant below has been omitted for simplicity):

$$|\Psi_{\lambda,N=1}\rangle=|1,0\rangle\pm|0,1\rangle, \quad (15a)$$

$$|\Psi_{\lambda,N=2}\rangle=|0,2\rangle+s|2,0\rangle+\delta_{s,+}\frac{\lambda}{\sqrt{2}}|1,1\rangle, \quad s=\pm, \quad (15b)$$

$$|\Psi_{\lambda,N=3}\rangle=|0,3\rangle+s|3,0\rangle+\frac{\lambda}{\sqrt{3}}(|1,2\rangle+s|2,1\rangle), \quad s=\pm, \quad (15c)$$

$$|\Psi_{\lambda,N=4}\rangle=|0,4\rangle+s|4,0\rangle+\frac{\lambda}{2}(|1,3\rangle+s|3,1\rangle)+\delta_{s,+}\frac{\lambda^2+6\tilde{g}\lambda-4}{2\sqrt{6}}|2,2\rangle, \quad s=\pm, \quad (15d)$$

$$|\Psi_{\lambda,N=5}\rangle=|0,5\rangle+s|5,0\rangle+\frac{\lambda}{\sqrt{5}}(|1,4\rangle+s|4,1\rangle)+\frac{\lambda^2+8\tilde{g}\lambda-5}{2\sqrt{10}}(|2,3\rangle+s|3,2\rangle), \quad s=\pm, \quad (15e)$$

$$|\Psi_{\lambda,N=6}\rangle=|0,6\rangle+s|6,0\rangle+\frac{\lambda}{\sqrt{6}}(|1,5\rangle+s|5,1\rangle)+\frac{\lambda^2+10\tilde{g}\lambda-6}{2\sqrt{15}}(|2,4\rangle+s|4,2\rangle)+\delta_{s,+}\frac{\lambda^3+26\tilde{g}\lambda^2+16(10\tilde{g}-1)\lambda-96\tilde{g}}{12\sqrt{5}}|3,3\rangle,\quad s=\pm, \tag{15f}$$

$$|\Psi_{\lambda,N=7}\rangle=|0,7\rangle+s|7,0\rangle+\frac{\lambda}{\sqrt{7}}(|1,6\rangle+s|6,1\rangle)+\frac{\lambda^2+12\tilde{g}\lambda-7}{2\sqrt{21}}(|2,5\rangle+s|5,2\rangle)+\frac{\lambda^3+32\tilde{g}\lambda^2+(240\tilde{g}^2-19)\lambda-140\tilde{g}}{6\sqrt{35}}(|3,4\rangle+s|4,3\rangle),\quad s=\pm. \tag{15g}$$

Equations (12) and (13) are suitable for the Hamiltonian (3), but they are equally suitable for the results of the Hamiltonian (1) after adding $-gN^2/2$ term to the right hand side (rhs) of Eq. (12a). Of course, the eigenkets $|n_1,n_2\rangle$ on the rhs of Eq. (12b) [suitable for both the Hamiltonians (1) and (3)] represent the Fock state of the operators $a_{1,2}$ (i.e., $a_1|n_1,n_2\rangle=\sqrt{n_1}|n_1-1,n_2\rangle$ and $a_2|n_1,n_2\rangle=\sqrt{n_2}|n_1,n_2-1\rangle$). Using $a_1\equiv -ia$ and $a_2\equiv b$, the results suitable for the Hamiltonian (1) can be written as follows:

$$E=gN(N-2)/2+\Omega\lambda, \tag{16a}$$

$$|\Psi_{\lambda,N}\rangle=\sum_{j=0}^{\mathrm{int}(N/2)}\frac{C}{1+\delta_{j,N/2}}\sqrt{\frac{(N-j)!}{N!j!}}\det W^{(j)}(\lambda)[(-i)^j|j,N-j\rangle_{ab}+(-i)^{N-j}s|N-j,j\rangle_{ab}], \tag{16b}$$

where $|n,k\rangle_{ab}=(1/\sqrt{n!k!})a^{\dagger n}b^{\dagger k}|0,0\rangle_{ab}$ denotes the Fock state of the operators a and b (i.e., $a|n,k\rangle_{ab}=\sqrt{n}|n-1,k\rangle_{ab}$ and $b|n,k\rangle_{ab}=\sqrt{k}|n,k-1\rangle_{ab}$), and both the matrices $W^{(j)}$ and the parameter λ are the same as those in Eq. (12).

IV. λ'S ANALYTICAL EXPRESSIONS

In the preceding section, we have explicitly given the analytical expressions of all the energy eigenstates in terms of the parameter λ determined by solving either analytically or numerically Eq. (13). Solving Eq. (13) is nothing but finding the roots of the polynomials either of the order of $N/2+1$ and $N/2$, respectively (for a positive even integer N), or of the order of $(N+1)/2$ (for a positive odd integer N). The explicit analytical expressions of the parameter λ for $N\leqslant 7$ can be readily obtained by a simple MATHEMATICA code. Once we substitute these analytical expressions for the parameter λ into Eq. (12), we immediately obtain the explicit analytical expressions of all the energy eigenvalues and eigenstates in terms of the given parameters Ω and g ($\tilde{g}\equiv g/\Omega$).

Although we can obtain the analytical results of the parameter λ for $N\leqslant 7$ by a simple MATHEMATICA code, here we only list those for $N\leqslant 5$ (λ for a fixed N is denoted as $\lambda^{(N)}$),

$$\lambda^{(1)}=s=\pm 1, \tag{17a}$$

$$\lambda^{(2)}=0\quad (s=-1),\quad \lambda^{(2)}=-\tilde{g}\pm\sqrt{4+\tilde{g}^2}\quad (s=1), \tag{17b}$$

$$\lambda^{(3)}=s-2\tilde{g}\pm 2\sqrt{1-s\tilde{g}+\tilde{g}^2},\quad s=\pm 1, \tag{17c}$$

$$\lambda^{(4)}=-3\tilde{g}\pm\sqrt{4+9\tilde{g}^2}\quad \text{as}\quad s=-1,$$

$$\lambda^{(4)}=\frac{-14\tilde{g}+4\sqrt{12+13\tilde{g}^2}\cos[(\theta+2\pi\xi)/3]}{3}\quad \text{as}\quad s=1,$$

$$\theta=\cos^{-1}\left[\frac{|35\tilde{g}^3-72\tilde{g}|}{(12+13\tilde{g}^2)^{3/2}}\right],\quad \xi=0,\pm \tag{17d}$$

$$\lambda^{(5)}=s\lambda_\xi^{(5)}(s\tilde{g}),\quad s=\pm 1,\quad \xi=0,\pm,$$

$$\lambda_\xi^{(5)}(\tilde{g})=\frac{3-20\tilde{g}+8\sqrt{7\tilde{g}^2-3\tilde{g}+3}\cos[(\theta'+2\pi\xi)/3]}{3},$$

$$\theta'=\cos^{-1}\left[\frac{|80\tilde{g}^3+18\tilde{g}^2-72\tilde{g}|}{8(7\tilde{g}^2-3\tilde{g}+3)^{3/2}}\right], \tag{17e}$$

where $\cos^{-1}$ denotes the principal value of the inverse cosine function.

V. RESULTS IN THE RABI AND FOCK REGIMES

In this section, we discuss the explicit forms for both the energy eigenvalues and eigenstates in the two regimes [21,22], i.e., the Rabi regime where $|\tilde{g}|\ll N^{-1}$ and the Fock regime where $|\tilde{g}|\gg N$.

A. Rabi regime's results

In the Rabi regime where $|\tilde{g}|\ll N^{-1}$, we can approximately take $\tilde{g}=0$ in the matrix elements $W_{ij}^{(s)}(\lambda)$ given by Eq. (14) and then use a MATHEMATICA code to solve Eq. (13) to obtain the following results:

$$\lambda\approx\pm(N-2n),\quad n=0,1,\ldots,\mathrm{int}(N/2). \tag{18}$$

Substituting these λ's values into Eq. (12), we immediately obtain explicitly the analytical expressions of all the energy eigenvalues and eigenstates in the Rabi regime. However, the explicit analytical expressions of the energy eigenstates for the parameter λ given by Eq. (18) can be most quickly ob-

tained by solving directly Eq. (8) with $\tilde{g}\approx 0$ (due to $|\tilde{g}| \ll N^{-1}$) by the simple MATHEMATICA code $\lambda=(N-2n)\ or\ -(N-2n);g=0;Dsolve[2gx^2y''[x]+(1-x^2-2(n-1)gx)y[x]==(\lambda-Nx)y[x],y[x],x]$ with the results

$$|\Psi_{\lambda\approx(N-2n)}\rangle = C_+(a_1^\dagger - a_2^\dagger)^n(a_1^\dagger + a_2^\dagger)^{N-n}|\text{vac}\rangle, \tag{19a}$$

$$|\Psi_{\lambda\approx-(N-2n)}\rangle = C_-(a_1^\dagger - a_2^\dagger)^{N-n}(a_1^\dagger + a_2^\dagger)^{n}|\text{vac}\rangle, \tag{19b}$$

where $C_\pm$ are normalization constants, $|\text{vac}\rangle$ denotes the vacuum state or the one without any atoms in both modes, and $n=0,1,\ldots,\text{int}(N/2)$. In particular, the maximum and minimum energy eigenvalues $E\approx gN(N-1)\pm\Omega N\approx\pm\Omega N$ (due to $|\tilde{g}|\ll N^{-1}$) and the corresponding energy eigenstates are

$$|\Psi_{\lambda\approx\pm N}\rangle \approx \frac{(a_1^\dagger \pm a_2^\dagger)^N}{\sqrt{2^N N!}}|\text{vac}\rangle. \tag{20}$$

When $\Omega>0$ (<0), the ground state is $|\Psi_{\lambda\approx -N}\rangle$ ($|\Psi_{\lambda\approx N}\rangle$).

B. Fock regime's results

In the Fock regime where $|\tilde{g}|\gg N$, it is readily shown from Eqs. (12) and (13) that all the energy eigenvalues and eigenstates can be written explicitly as follows:

$$E_n = g[N(N-1)-2n(N-n)]+s\Omega(N+1)\delta_{n,(N-1)/2} + \mathcal{O}\left(\frac{1}{\tilde{g}^2}\right), \tag{21a}$$

$$|\Psi_n\rangle = C'\sum_{j=0}^{j_{max}} \frac{(-2\tilde{g})^{j-n}(N-2n)!\sqrt{(N-j)!n!}}{(N-n-j)!\sqrt{j!(N-n)!}(1+\delta_{j,N/2})}(|j,N-j\rangle + s|N-j,j\rangle), \tag{21b}$$

where $s=\pm 1$, $j_{max}=\max\{\text{int}(N/2),n\}$, $n=0,1,\ldots,\text{int}(N/2)$, and C' is a normalization constant. Equation (21b) explicitly describes how the energy eigenstates vary with respect to variable $\tilde{g}$ in the Fock regime where $|\tilde{g}|\gg N$.

It is instructive to note that the ground state(s) under the conditions $|\tilde{g}|=\infty$ (or $\Omega=0$) and $g>0$ becomes

$$|\Psi_{gr}\rangle = \left|\frac{N}{2},\frac{N}{2}\right\rangle, \quad s=1, \quad N=\text{even}, \tag{22a}$$

$$|\Psi_{gr}\rangle = \frac{1}{\sqrt{2}}\left(\left|\frac{N-1}{2},\frac{N+1}{2}\right\rangle + s\left|\frac{N+1}{2},\frac{N-1}{2}\right\rangle\right), \quad s=\pm 1, \quad N=\text{odd}. \tag{22b}$$

Expression (22) demonstrates that there are two ground states (corresponding to $s=1$ and $s=-1$, respectively) when N is an odd positive integer, while there exists only a unique ground state when N is an even positive integer. However, it is emphasized that this kind of ground-state degeneracy when N is an odd positive integer exists only under the conditions $|\tilde{g}|=\infty$ (or $\Omega=0$) and $g>0$ and it does not exist at all when $|\tilde{g}|\to\infty$ but with $\Omega\neq 0$, because only the case $s=-1$ in Eq. (22b) is the unique ground state for $\Omega\neq 0$, which can be readily seen from Eq. (21) although the energy of state (22b) for $s=1$ is very near the ground-state energy when $|\tilde{g}|\to\infty$ but with $\Omega\neq 0$.

It is interesting to note from Eqs. (20) and (22) that the ground states in the Rabi and Fock regimes have dramatically different phase behaviors. In the Fock regime, the system's ground state given in Eq. (22) is a Fock state (the state with a fully incoherent phase) for an even positive integer N, and nearly so for an odd positive N at least for large N's; while in the Rabi regime, the ground state given by one of the states in Eq.(20) is a state with a fully coherent phase.

VI. CONCLUSIONS

In summary, we have presented an efficient and simple method to solve model (1) or (3) based on our previously developed approach. We have shown that all the energy eigenvalues and eigenstates for an arbitrary (small or large) total atom number N can be explicitly expressed analytically in terms of a parameter λ whose values can be obtained by finding the roots of at most two polynomials of at most of the order of $1+\text{int}(N/2)$. To be more specific, we need to find the roots of two polynomials of the order of $N/2+1$ and $N/2$, respectively for an even N and both of the order of $(N+1)/2$ for an odd N, but just as we have shown in the Appendix that we only need to find the roots of one of the two polynomials for an odd N. As explained below, the method and the results here are not only of theoretical interests in their own right but also may find wide applications in the fields of Bose-Einstein condensates, quantum optics, quantum information, and quantum computation.

First of all, the method is shown to have wide applicability to nonlinear processes in various fields of physics [15–19].

Second, in handling the systems with nonlinear interactions among several boson modes, one usually needs to make the so-called Bethe ansatz [20] on the energy eigenstates with several parameters determined by highly complicated reduced system of Bethe equations [20]. However, we have obtained the explicit analytical expressions of *all* the energy eigenstates in terms of a parameter λ for an arbitrary (small or large) total atom number N for model (1) or (3) considered here. These expressions are exact results without making any assumption particular without the so-called Bethe ansatz. Besides, the *single* parameter λ is determined by finding the roots of two polynomials of at most of the order of $1+\text{int}(N/2)$, which is much simpler than the usually complicated reduced system of Bethe equations for several parameters.

Third, dealing with the problem at hand is greatly simplified for small N cases and particularly for huge N as well, since we have reduced solving eigenvalue problem for a

$(N+1)\times(N+1)$ matrix A into finding the roots of at most two polynomials of at most of the order of $1+\mathrm{int}(N/2)$ to give all the energy eigenvalues and eigenstates.

Fourth, we can obtain the explicit analytical expressions of the parameter λ for $N\leqslant 7$ by a simple MATHEMATICA code [although we have listed them in Eq. (17) only for $N\leqslant 5$], and hence obtain via Eq. (12) the explicit analytical expressions of all the energy eigenvalues and eigenstates in terms of the known parameters Ω and g described in Eq. (1) or (3). The average occupations per well (site) in the experiment is around one to three atoms, which could potentially form elementary building blocks for atomic qubit based quantum computing designs [2,3], but no one seems to have been able to solve for the combined dynamics analytically even for a small number of atoms for such a system [3,6,7]. Therefore, the explicit analytical expressions of all the energy eigenvalues and eigenstates either in terms of the known parameters Ω and g for $N\leqslant 7$ or in terms of the parameter λ for other numbers of total atoms might be useful for preparation, manipulation, and control of a Bose-Einstein condensate in optical lattices in a Mott-insulator state or of a double-well Bose-Einstein condensate, and for facilitating the investigation of massive maximum entangled pairs, triplets, quartiles, and other clusters of Bose condensed atoms in such systems.

Finally, the exact analytical results in the present paper are expected to play a role in checking the applicable range of various approximations such as the number-conserving Bogoliubov theory [11,12].

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APPENDIX

In this appendix, we show Eqs. (12b), (13), and (14) in the main text. Let us show them for the cases of odd and even integers N separately.

1. The odd N case

In this case, the column vectors in Eq. (11) have the form $\alpha=(\alpha_0,\alpha_1,\ldots,\alpha_{(N-1)/2},s\alpha_{(N-1)/2},\ldots,s\alpha_1,s\alpha_0)^T$ with $s=\pm$ and $f(z)=\sum_{j=0}^{(N-1)/2}\alpha_j(z^j+sz^{N-j})$. Substituting $\alpha=(\alpha_0,\alpha_1,\ldots,\alpha_{(N-1)/2},s\alpha_{(N-1)/2},\ldots,s\alpha_1,s\alpha_0)^T$ into Eq. (10) and introducing $\gamma_j=j!\alpha_j$, we obtain

$$\gamma_{j+1}=a_j^{(s)}(\lambda)\gamma_j-p_{j-1}\gamma_{j-1},\quad 0\leqslant j\leqslant q, \tag{A1}$$

where $q=\mathrm{int}(N/2)\equiv(N-1)/2$ for positive odd integers N, $\gamma_{-1}=\gamma_{(N+1)/2}=0$, $p_j=(j+1)(N-j)$, and $a_j^{(s)}(\lambda)=\lambda-2\tilde{g}j(j-N)-s(N+1)\delta_{j,(N-1)/2}/2$. This set of equations can be put into the form

$$W^{(s,q+1)}(\lambda)\gamma=0, \tag{A2}$$

where the column vector $\gamma=(\gamma_0,\gamma_1,\ldots,\gamma_q)^T$. We introduce the matrices $W^{(s,j)}$ as $W^{(s,0)}(\lambda)\equiv 1$, where $W^{(s,k)}(\lambda)$ $(k\geqslant 1)$ is a $k\times k$ trigonal matrix with the matrix elements $W_{ij}^{(s,k)}(\lambda)=a_j^{(s)}(\lambda)\delta_{i,j}-\delta_{i+1,j}-p_{i-1}\delta_{i,j+1}$ $(i,j=0,1,\ldots,k-1)$. Equation (A2) with $\gamma\neq 0$ immediately leads to

$$\det W^{(s,q+1)}(\lambda)=0,\quad s=\pm,\quad q=\mathrm{int}(N/2). \tag{A3}$$

Besides, it is readily shown that

$$\alpha_j=\frac{\alpha_0}{j!}\det W^{(s,j)}(\lambda),\quad j=0,1,2,\ldots,q. \tag{A4}$$

The proof of Eq. (A4) is as follows. Expanding the $(n+1)\times(n+1)$ trigonal determinant $\det W^{(s,n+1)}$ by the $(n+1)$th column leads to $\det W^{(s,n+1)}=a_n^{(s)}(\lambda)\det W^{(s,n)}+K$, where K is an $n\times n$ determinant obtained by deleting both the nth row and $(n+1)$th column of the determinant $\det W^{(s,n+1)}$. Obviously, there exists only one nonzero element $-p_{n-1}$ in the last row of the determinant K and hence $K=-p_{n-1}\det W^{(s,n-1)}$. Consequently, $\det W^{(s,n+1)}=a_n^{(s)}\det W^{(s,n)}-p_{n-1}\det W^{(s,n-1)}$ so that $\det W^{(s,j)}(\lambda)$ satisfy the same iterating equation (A1) as γ_k/γ_0. Equation (A4) is now obviously true by further noting the fact that $\det W^{(s,0)}(\lambda)\equiv 1$, $\det W^{(s,1)}(\lambda)=a_0^{(s)}$, and $\gamma_j=\alpha_j/j!$ $(\gamma_0=\alpha_0)$. Besides, noting the facts that $W^{(s,k)}(\lambda)\equiv W^{(k)}(\lambda)$ for $k\leqslant\mathrm{int}(N/2)\equiv(N-1)/2$ [since $-s(N+1)\delta_{j,(N-1)/2}/2$ in $a_j^{(s)}(\lambda)$ is zero due to $\delta_{j,(N-1)/2}/2=0$ when $j=0,1,\ldots,k-1$ as $k\leqslant\mathrm{int}(N/2)\equiv(N-1)/2$] and that $W^{(s,q+1)}(\lambda)\equiv W^{(s)}(\lambda)$ for positive odd integers N since $p_j^{(s)}=(j+1)[(N-j)+\delta_{s,+}\delta_{j+1,N/2}(N/2+1)]\equiv p_j=(j+1)(N-j)$ due to $\delta_{j+1,N/2}=0$ for the odd N case, Eqs. (A3) and (A4), together with Eqs. (9) and (11), result in Eqs. (12) and (13) in the main text for the odd N case.

Besides, for the odd N case, only the roots of one of the two polynomials in Eq. (13) or (A3) are needed to be found to give all the λ's values. This conclusion can be readily shown as follows. Let us denote $W^{(\pm)}(\lambda)$ as $W^{(\pm)}(\lambda,\tilde{g})$ to explicitly illustrate their dependence on the parameter $\tilde{g}$. Then using the expression of the matrices $W^{(\pm)}(\lambda,\tilde{g})$ given after Eq. (14), it is readily shown that $W^{(+)}(-\lambda,-\tilde{g})=-QW^{(-)}(\lambda,\tilde{g})Q^{-1}$ for the odd N case. Here $Q^{-1}\equiv Q$ is a diagonal matrix with elements $Q_{ij}=(-1)^i\delta_{i,j}$ $(i,j=0,1,\ldots,(N-1)/2)$. Consequently, we have $\det W^{(-)}(\lambda,\tilde{g})=(-1)^{(N+1)/2}\det W^{(+)}(-\lambda,-\tilde{g})$ by noting $(\det Q)(\det Q^{-1})=\det(QQ^{-1})=1$. This proves the conclusion.

2. The even N case

When N is an arbitrary positive even integer ($N=0$ is a trivial case and hence is excluded hereafter), Eq. (11) gives the constraint $(s-1)\alpha_{N/2}=0$ or $\alpha_{N/2}=0$ for $s=-1$. Consequently, for $s=-1$, column vectors in Eq. (11) have the form $\alpha=(\alpha_0,\alpha_1,\ldots,\alpha_{N/2-1},0,-\alpha_{N/2-1},\ldots,-\alpha_1,-\alpha_0)^T$ and hence $f(z)=\sum_{j=0}^{N/2-1}\alpha_j(z^j-z^{N-j})$. For $s=1$, we have $\alpha=(\alpha_0,\alpha_1,\ldots,\alpha_{N/2-1},\alpha_{N/2},\alpha_{N/2-1},\ldots,\alpha_1,\alpha_0)^T$ and $f(z)=\sum_{j=0}^{N/2-1}\alpha_j(z^j+z^{N-j})+\alpha_{N/2}z^{N/2}$. It is pointed out

that $f(z)$ for both $s=1$ and $s=-1$ can be written as $f(z)=\sum_{j=0}^{N/2}[\alpha_j(z^j+sz^{N-j})/(1+\delta_{j,N/2})]$ because of $z^j+sz^{N-j}=0$ when $s=-1$ and $j=N/2$. Substituting $\alpha=(\alpha_0,\alpha_1,\ldots,\alpha_{N/2-1},0,-\alpha_{N/2-1},\ldots,-\alpha_1,-\alpha_0)^T$ $(s=-1)$ or $\alpha=(\alpha_0,\alpha_1,\ldots,\alpha_{N/2-1},\alpha_{N/2},\alpha_{N/2-1},\ldots,\alpha_1,\alpha_0)^T$ $(s=1)$ into Eq. (10) and again introducing $\gamma_j=j!\,\alpha_j$, we obtain from Eq. (10) the results

$$\gamma_{j+1}=a_j(\lambda)\gamma_j-p_{j-1}^{(s)}\gamma_{j-1},\quad 0\leqslant j\leqslant q^{(s)}, \tag{A5}$$

where $q^{(s)}=\mathrm{int}(N/2)-\delta_{s,-}$, $\gamma_{-1}=\gamma_{q^{(s)}+1}=0$, $a_j(\lambda)=\lambda-2\tilde{g}j(j-N)$, and $p_j^{(s)}=(j+1)[(N-j)+\delta_{s,+}\delta_{j+1,N/2}(N/2+1)]$. This set of equations can also be put into the form $W^{(s,q^{(s)}+1)}(\lambda)\gamma=0$ with the column vector $\gamma=(\gamma_0,\gamma_1,\ldots,\gamma_{q^{(s)}})^T$. The matrices $W^{(s,j)}$ in this even N case are defined as $W^{(s,0)}(\lambda)\equiv 1$, where $W^{(s,k)}(\lambda)$ $(k\geqslant 1)$ is a $k\times k$ trigonal matrix with the matrix elements $W_{ij}^{(s,k)}(\lambda)=a_j(\lambda)\delta_{i,j}-\delta_{i+1,j}-p_{i-1}^{(s)}\delta_{i,j+1}$ $(i,j=0,1,\ldots,k-1)$. It is now straightforward to follow the same routine as we did for the odd case to show that for the even case, we have

$$\det W^{(s,q^{(s)}+1)}(\lambda)=0,\quad s=\pm,\quad q^{(s)}=\mathrm{int}(N/2)-\delta_{s,-}, \tag{A6}$$

$$\alpha_j=\frac{\alpha_0}{j!}\det W^{(j)}(\lambda),\quad 0\leqslant j\leqslant q^{(s)}. \tag{A7}$$

Once again we have made use of the identities $W^{(s,k)}(\lambda)\equiv W^{(k)}(\lambda)$ for $0\leqslant k\leqslant q^{(s)}$, since $\delta_{j+1,N/2}=0$ in $p_j^{(s)}=(j+1)[(N-j)+\delta_{s,+}\delta_{j+1,N/2}(N/2+1)]$ when $j\leqslant(k-1)\leqslant(q^{(s)}-1)$. In addition, $W^{(s,q^{(s)}+1)}(\lambda)\equiv W^{(s)}(\lambda)$ due to $a_j^{(s)}(\lambda)=\lambda-2\tilde{g}j(j-N)-s(N+1)\delta_{j,(N-1)/2}/2\equiv a_j(\lambda)$ $(\delta_{j,(N-1)/2}=0)$ for the even N case. It is noted that $j=N/2=q^{(-)}+1$ for $s=-$ can be included in Eq. (A7) because $\det W^{(N/2)}(\lambda)\equiv\det W^{(-,N/2)}(\lambda)=0$ so that the included $\alpha_{N/2}=0$ for $s=-$ as it should be. Eqs. (A6) and (A7) (after including $j=N/2=q^{(-)}+1$ for $s=-$), together with Equations (9) and (11), result in Eqs. (12) and (13) in the main text for the even N case.

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