Analytical solutions for two heteronuclear atoms in a ring trap

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We consider two heteronuclear atoms interacting with a short-range δ potential and confined in a ring trap. By taking the Bethe-ansatz-type wavefunction and considering the periodic boundary condition properly, we derive analytical solutions for the heteronuclear system. The eigen-energies represented in terms of quasi-momentums can then be determined by solving a set of coupled equations. We present a number of results, which display different features from the case of identical atoms. Our result can be reduced to the well-known Lieb-Liniger solution when two interacting atoms have the same masses.

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I. INTRODUCTION

Motivated by recent experimental studies on heteronuclear atoms, mixtures of atomic gas with different masses have recently attracted lots of attention. Stable mixtures of heteronuclear atoms, for examples, 40K and 6Li, 40K and 87Rb, and 6Li and 23Na, have already been realized in experiments [1–6]. The heteronuclear quantum gas mixture offers a wide range of possibilities for exploring novel phases and new quantum effects. Significant efforts have been made on research topics such as superfluid properties and pairing mechanisms of heteronuclear fermions [7–9] and heteronuclear molecule formation [10,11].

The mass ratio between heteronuclear atoms adds a new degree of freedom for exploring physical effects associated with the mass imbalance. In general, heteronuclear atomic systems are expected to behave quite differently than the equal-mass counterpart [7–9,12–14]. To gain deep insight into properties of heteronuclear systems, some analytical solutions are especially important. While most of theoretical works on the many-body heteronuclear systems are within the mean-field theory, few-body systems can be treated much more precisely within nonperturbative microscopic frameworks [14]. Particularly, the two-body problem is vital to understand the basic physical phenomenon from the beginning of quantum mechanics. The two-atom system composed of identical atoms is exactly solved as one can separate the center-of-mass and relative motions and thus the two-particle system turns to a one-body problem [12] [13]. The problem with different atoms becomes complicated and generally is hard to get analytical solutions as it does not separate in center-of-mass and relative coordinates [12]. Recently, the scattering of heteronuclear atom pairs in a one-dimensional optical lattice has been studied by using the method of Green’s function [20].

In this article, we study the problem of two unequal-mass atoms with δ-potential interaction in a one-dimensional ring trap with periodic geometry. The periodic geometry has been experimentally realized as a circular wave guide or toroidal trap [21,22]. For the two-atom system with δ-potential interaction, it is convenient to treat the interaction term by separating center-of-mass and relative motion. However, it is not convenient to apply the periodic boundary condition by using separated center of mass and relative coordinates. When the periodic boundary condition is taken into account, the relative motion is actually coupled to the center-of-mass motion. In the present work, we analytically solve the problem of interacting two heteronuclear atoms by taking the Bethe-ansatz-type wavefunction and considering the periodic boundary condition properly. While the momentum of center-of-mass motion is a good quantum number, the relative momentum is coupled to the center-of-mass momentum due to the periodic boundary condition. Our results are consistent with the exact Bethe-ansatz solutions of the Lieb-Liniger model when two atoms have the same mass [18].

momentum due to the periodic boundary condition. Our results are consistent with the exact Bethe-ansatz solutions of the Lieb-Liniger model when two atoms have the same mass [18]. With the analytical solution, we obtain the energy spectrum, density distribution and momentum distribution for different mass ratio. Our results indicate that they display different features from the identical two-atom system.

The paper is organized as follows: In Sec.II, we introduce the model and present a detailed derivation of the analytical solution of the interacting heteronuclear system. In the limit of equal mass, our analytical result is compared to the Bethe-ansatz solution of two-particle Lieb-Liniger model. In Sec.III, we present the energy spectrum of heteronuclear atoms. In Sec.IV, we show the density distribution of relative coordinate and the momentum distribution of heteronuclear atoms. A summary is given in the last section.

II. THE MODEL AND ITS SOLUTIONS

We consider an interacting two-atom system in a 1D ring trap described by the Hamiltonian

\[ \hat{H} = -\frac{\hbar^2}{2m_1} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2} \frac{\partial^2}{\partial x_2^2} + g\delta(x_1 - x_2), \] (1)
where \( g \) is the interaction strength and the general case with different masses \( m_1 \) and \( m_2 \) is considered. The geometry of the ring trap enforces the periodic boundary condition

\[
\Psi(x + L, x_2) = \Psi(x, x_2 + L) = \Psi(x, x_2)
\]  
(2)

to the eigenfunction \( \Psi(x_1, x_2) \) of Hamiltonian \( \hat{H} \). Introducing relative and center-of-mass coordinates \( x = x_1 - x_2, \tilde{X} = (m_1x_1 + m_2x_2)/(m_1 + m_2) \), or alternatively \( x_1 = \tilde{X} + \frac{m_2}{m_1 + m_2}x_2, x_2 = \tilde{X} - \frac{m_1}{m_1 + m_2}x_2 \), we can rewrite the Hamiltonian Eq. (1) as the separated form

\[
\hat{H} = \hat{H}_{X}(X) + \hat{H}_{x}(x)
\]

\[
= -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial X^2} - \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial x^2} + g\delta(x),
\]
(3)

where \( \mu = m_1m_2/(m_1 + m_2) \) and \( M = m_1 + m_2 \). The wavefunctions of the Hamiltonian can take the form of \( \Psi(X, x) = e^{ikX} \phi(x) \), where \( e^{ikX} \) is the eigenstate of \( \hat{H}_{X}(X) \) and the eigenstate of \( \hat{H}_{x}(x) \) has the form of

\[
\phi(x) = (A_+ e^{ikx} + B_+ e^{-ikx})\theta(x) + (A_- e^{ikx} + B_- e^{-ikx})\theta(-x),
\]
(4)

where \( A_+ \) and \( B_+ \) are coefficients to be determined. It is straightforward to get the eigenenergy given by

\[
E = \frac{\hbar^2}{2M}k^2 + \frac{\hbar^2}{2\mu}k^2.
\]
(5)

Although formally the center-of-mass and relative parts are separated, we shall show that the relative quasi-momentum \( k \) is actually coupled with the total momentum \( K \) due to the periodic boundary condition (2).

The continuous condition of the wavefunction (4) gives the following restriction to the coefficients:

\[
A_+ + B_+ = A_- + B_-.
\]
(6)

By integrating the eigen-equation \( \hat{H}\Psi(X, x) = E\Psi(X, x) \) from the negative infinitesimal \( -\epsilon \) to the positive infinitesimal \( \epsilon \), we get

\[
-\frac{\hbar^2}{2\mu} \left( \frac{\partial}{\partial x} \phi(x)_{x = \epsilon} - \frac{\partial}{\partial x} \phi(x)_{x = -\epsilon} \right) + g\phi(0) = 0,
\]

which leads to

\[
\alpha k(A_+ - B_+) = \alpha \frac{\mu}{\hbar^2} g(A_+ + B_+ + A_- + B_-).
\]
(7)

The Eq. (10) and Eq. (7) can not uniquely determine all the parameters. Additional relations can be obtained by considering the periodic boundary condition (2). In order to apply the periodic boundary condition, it is more convenient to work in the coordinate space of \( x_1 \) and \( x_2 \). In terms of \( x_1 \) and \( x_2 \), the total wavefunction \( \Psi(x_1, x_2) = \Psi(X, x) = e^{ikX} \phi(x) \) can be also represented as

\[
\Psi(x_1, x_2) = (A_+ e^{ik_1x_1 + ik_2x_2} + B_+ e^{ik_1'x_1 + ik_2'x_2})\theta(x_1 - x_2) + (A_- e^{ik_1x_1 + ik_2x_2} + B_- e^{ik_1'x_1 + ik_2'x_2})\theta(x_2 - x_1),
\]
(8)

where \( k_1 = Km_1/(m_1 + m_2) + k, k_2 = Km_2/(m_1 + m_2) - k, k_1' = Km_1/(m_1 + m_2) - k, k_2' = Km_2/(m_1 + m_2) + k \). The periodic boundary condition then enforces

\[
A_+ e^{ik_1L} = A_-, \quad (9)
\]
\[
B_+ e^{ik_2' L} = B_-,
\]
(10)
\[
A_- e^{ik_2L} = A_+,
\]
(11)
\[
B_- e^{ik_2' L} = B_+.
\]
(12)

By multiplying Eqs. (9) and (11) or Eqs (10) and (12), we get \( e^{ikL} = 1 \), which implies

\[
KL = 2\pi n, \quad (13)
\]

with \( n \) the integer. Combining Eqs. (9) (10) and (6), we can represent \( B_+ \), \( A_+ \), \( B_- \) in terms of \( A_+ \). Substituting them into Eq. (7), we can derive the following relation

\[
\frac{\hbar^2}{\mu g} = \frac{\sin(kL)}{\cos(Km_1/km_2) - \cos(kL)}. \quad (14)
\]

From Eq. (14), it is clear that \( k \) is coupled with the \( K \) whereas \( K \) is uniquely determined by Eq. (13). By solving Eqs. (13) and (14), we can get solutions of \( k \) and \( K \) and therefore eigenvalues of the system by Eq. (5).

The above equations can be also represented in terms of the quasi-momentum \( k_1 \) and \( k_2 \) via \( K = k_1 + k_2 \) and \( k = (m_2k_1 - m_1k_2)/(m_1 + m_2) \). In terms of \( k_1 \) and \( k_2 \), the eigenenergy is given by

\[
E = \frac{\hbar^2}{2m_1}k_1^2 + \frac{\hbar^2}{2m_2}k_2^2. \quad (15)
\]

In order to compare to the case with the same masses, we introduce \( g = \frac{\hbar^2}{m_1c} \) and rewrite Eq. (14) as

\[
\left( 1 + \frac{1}{\alpha} \right) \frac{k}{c} = \frac{\sin(kL)}{\cos(Km_1/km_2) - \cos(kL)}, \quad (16)
\]

where \( \alpha = m_2/m_1 \) is the mass ratio. When the mass ratio \( \alpha = 1 \), our results (13) and (14) should be consistent with the well-known Bethe-ansatz solution of the Lieb-Liniger model (18). Using the above relation (16) and taking \( \alpha = 1 \), we can get

\[
\frac{2k + ic}{2k - ic} = \frac{e^{ikL} - \cos(KL/2)}{e^{ikL} - \cos(KL/2) - e^{-ikL}}.
\]

Since \( \cos(KL/2) = \cos(\pi n) = \pm 1 \), the above equation reduces to

\[
k_1 - k_2 + ic = \pm e^{ikL},
\]

where \( + \) (or \( - \)) corresponds to \( n = \text{even} \) (or odd). By using the relation \( e^{ikL} = e^{i(k_1 - k_2)L/2} = e^{ik_1L}e^{-iK/2} = \pm e^{ik_1L} \), we then have

\[
e^{ikL} = \frac{k_1 - k_2 + ic}{k_1 - k_2 - ic}. \quad (17)
\]
which is just the Bethe-ansatz equation of the two-particle Lieb-Liniger model \cite{18}. Another Bethe-ansatz equation can be obtained via \( e^{ik_2L} = e^{-ik_1L} \). When \( n_1 = m_2 \), we have \( k'_1 = k_2 \) and \( k'_2 = k_1 \). From Eqs. (10) and (6), we can also get \( A_+ = B_+ \) and \( B_- = A_- \). Therefore the wavefunction also has the same form of the Lieb-Liniger model \cite{18}, which is invariant under the the exchange of \( x_1 \) and \( x_2 \). We note that, for the general case with mass imbalance, the wavefunction is not invariant under the exchange of \( x_1 \) and \( x_2 \) since \( k'_1 \neq k_2 \) and \( k'_2 \neq k_1 \).

### III. THE ENERGY SPECTRUM

Without loss of generality, only the case of \( \alpha \geq 1 \) shall be considered. For convenience, in the following calculation we shall take \( \hbar = 1 \) and \( 2m_1 = 1 \). In the units of energy \( \hbar^2/(2m_1) = 1 \), the energy expression Eq. (5) or Eq. (15) becomes

\[
E = (1 + \alpha)^{-1} K^2 + (1 + 1/\alpha) k^2
\]

or \( E = k_1^2 + (1/\alpha) k_2^2 \). Since the total momentum \( K \) is a conserved quantity determined by Eq. (13), the energy spectrum of the system \( E \) can be characterized by different \( K \). The ground state corresponds to \( K = 0 \). Given \( K = 2\pi n/L \), \( k \) can be determined by solving Eq. (14) or Eq. (16). For the repulsive case with \( c > 0 \), Eq. (16) has only real solutions which describe the scattering states. However, for the attractive case with \( c < 0 \), Eq. (16) may have imaginary solutions corresponding to the bound states of the attractive system.

First we shall consider the case with the total momentum \( K = 0 \). For \( K = 0 \), Eq. (16) becomes

\[
\left( 1 + \frac{1}{\alpha} \right) \frac{k}{c} = \frac{\sin(kL)}{1 - \cos(kL)}
\]

With similar steps as the equal-mass case, we can get

\[
e^{ikL} = \frac{k + ic'}{k - ic'}
\]

with \( c' = c/\left(1 + \frac{1}{\alpha}\right) \). For \( c > 0 \), \( k \) has only real solutions. It is convenient to solve the real solution of \( k \) from the logarithm form of Eq. (19) given by

\[
kL = 2\pi (I - 1/2) - 2 \arctan(k/c'),
\]

where \( I \) takes integer. By numerically solving the \( k \) solution, we can get the energy \( E = (1 + 1/\alpha) k^2 \) for states with \( K = 0 \). The ground state energy corresponds to the solution of Eq. (20) with \( I = 1 \). For \( c < 0 \), Eq. (19) has imaginary solution \( k = i\lambda \). The real solution \( \lambda \) can be obtained by solving

\[
e^{-i\lambda L} = \frac{\lambda + c'}{\lambda - c'}
\]

which is obtained by inserting \( k = i\lambda \) into Eq. (19). From Eq. (21), one can also check that \( \lambda \) has only solution for \( c' < 0 \). The energy of the bound state can be obtained via \( E = -(1 + 1/\alpha) \lambda^2 \).

To give a concrete example, we consider a two-atom system composed of \( ^{40} \)K and \( ^{87} \)Rb with the mass ration \( \alpha = 2.175 \). In Fig.1, we plot the energy spectrum for states with \( K = 0 \). The energy spectrum for \( \alpha = 2.175 \) is represented by dashed lines. The energy spectrum of the equal-mass system is also given for comparison. Here we use the dimensionless energy \( \epsilon(\gamma) = E/N(\rho^2) \), where \( \rho = N/L \) and \( N = 2 \) is the atom number. It is shown that the ground energy for the system of \( \alpha > 1 \) has lower energy than that of the system with \( \alpha = 1 \). Actually, all the other spectrum corresponding to quantum number \( I \) for \( \alpha > 1 \) is below its correspondence for \( \alpha = 1 \).

Now we consider states with the nonzero total momentum, for example, \( K = \pm \frac{2\pi}{L} \), which correspond to excited states of the system. When \( K \neq 0 \), Eq. (16) cannot be simplified to a similar form as Eq. (19) or Eq. (20) for an arbitrary \( \alpha \). Nevertheless, formally we have

\[
kL = 2\pi I - 2 \arctan \frac{k}{c'} - 2 \arctan \left[ \frac{kL}{2} \cot^2 \left( \frac{KL}{2(1 + \alpha)} \right) \right],
\]

where \( I \) takes integer. When \( K = 0 \), it reduces to Eq. (20). The relative momentum can be obtained by numerically solving Eq. (16) or (22) with \( K = \pm \frac{2\pi}{L} \) and the energy is given by \( E = (1 + \alpha)^{-1} \left( \frac{2\pi}{L} \right)^2 + (1 + 1/\alpha) k^2 \). The energies for \( K = 2\pi/L \) and \( K = -2\pi/L \) are degenerate. In Fig.2, we display energy spectrums of states with \( K = \pm 2\pi/L \) for \( \alpha = 2.175 \) and \( \alpha = 1 \). It is shown that the energy spectrum for \( \alpha > 1 \) is always below the corresponding spectrum for \( \alpha = 1 \).

The effect of mass ratio on energy spectrum can be understood from two aspects. First, we can see that coe-

![Fig. 1](image-url) (Color online) The dimensionless energy spectrum versus \( \gamma \) for \( K = 0 \), \( \alpha = 2.175 \) (dashed line) and \( \alpha = 1 \) (solid line). For \( \gamma < 0 \), there exists a bound state.
coefficients in Eq. (18) decrease as the mass ratio $\alpha$ increases. On the other hand, while $K$ in Eq. (18) is independent of the mass ratio, $k$ is related with $\alpha$ via the nonlinear equation (16). It is not easy to analytically analyze the influence of the mass ratio on $k$ from Eq. (16). However, for the case of $K = 0$, from Eq. (19) or Eq. (20), we notice that the mass ratio $\alpha$ affects the solution of $k$ by effectively changing the interaction strength via $c'$ and thus $k$ increases with the increase in $\alpha$.

For the attractive case with $c < 0$, it is worthy of indicating that there exists a bound state for each set of states characterized by $K$ when the interaction exceeds a threshold $c_t$. The threshold of $\gamma_t = c_t/\rho$ for the appearance of bound state is given by

$$\gamma_t = \frac{1}{2} \left( 1 + \frac{1}{\alpha} \right) \left[ \cos \left( \frac{KL}{1 + \alpha} \right) - 1 \right]. \quad (23)$$

For $K = 0$, we have $\gamma_t = 0$. This implies that the atoms form bound state for arbitrary weak attraction $\gamma < 0$. For $K = 2\pi/L$, we have $\gamma_t < 0$. In this case, atoms can form bound state only for $\gamma < \gamma_t$.

**IV. DENSITY AND MOMENTUM DISTRIBUTION**

To show the influence of the interaction on the wavefunction, we plot the ground state density distribution for the relative motion defined as $\rho(x) = \varphi^*(x)\varphi(x)$ in Fig. 4. The density distribution displays a cusp at $x = 0$ due to the repulsive interaction when two atoms coincide. The relative motion density distribution at $x = 0$ decreases as the interaction strength increases. The density distribution at $x = 0$ for the case of $\alpha > 1$ is below that of the equal-mass case as a consequence of increasing $c'$ effectively. In the limit of $c \to \infty$, the wave function $\Psi(x_1, x_2)$ vanishes whenever $x_1 = x_2$.

The momentum distribution for atom with mass $m_1$ can be represented as

$$n_1(p) = \int \Psi^*(p_1, p_2)\Psi(p_1, p_2)dp_2,$$

where $\Psi(p_1, p_2)$ is the Fourier transformation of $\Psi(x_1, x_2)$. The definition of momentum distribution $n_2(p)$ for the atom with mass $m_2$ is similar. For the equal-mass case, the momentum distribution for atom 1 or 2 should be the same since the wave function $\Psi(x_1, x_2)$ is invariant under the exchange of $x_1$ and $x_2$. However, the unequal-mass atomic system will show different features since the wave functions are not necessary to be symmetrical for exchanging two unequal mass atoms except of the case of $K = 0$. For $K = 0$, we find that the wavefunction is invariant under exchange of $x_1$ and $x_2$ even for the unequal-mass case, and thus we have $n_1(p) = n_2(p)$. In Fig. 4, we display the ground state momentum distribution for the unequal-mass system with $\alpha = 2.175$ and the equal-mass system. An obvious peak around the zero momentum position can be observed. With the increase in the interaction strength, the momentum distribution tends to spread out widely and the height of the peak decreases. There is no obvious difference for momentum distributions of systems with $\alpha = 2.175$ and $\alpha = 1$ as the influence of $\alpha$ can be attributed to the effective interaction $c'$.

Next we discuss the momentum distribution for the lowest state with $K = \pm 2\pi/L$. For these cases, unequal mass will have significant impact on the wavefunction and momentum distribution as the wave functions are not

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**FIG. 2:** (Color online) The dimensionless energy spectrum versus $\gamma$ for $K = \pm 2\pi/L$, $\alpha = 2.175$ (dashed line) and $\alpha = 1$ (solid line).

**FIG. 3:** (Color online) The probability density distribution of relative motion for the ground state with $\gamma = 1$ and $\alpha = 1$ (dash dot line), $\gamma = 1$ and $\alpha = 2.175$ (dashed line), $\gamma = 5$ and $\alpha = 1$ (short dashed line), $\gamma = 5$ and $\alpha = 2.175$ (dashed dotted dot line), $\gamma = 500$ and $\alpha = 1$ (short dashed dotted line), $\gamma = 500$ and $\alpha = 2.175$ (red dotted).
The momentum distributions become broader and the height of the main peak shrinks. As a comparison, in Fig. 6 we display the momentum distribution for the lowest states of the equal-mass systems with $K = \pm 2\pi/L$. Due to the exchange symmetry of the wave function, the momentum distributions $n_1(p) = n_2(p)$ when $m_1 = m_2$. For $K = 2\pi/L$, the momentum distribution displays two peaks around 0 and $2\pi/L$, while the distribution has two peaks around 0 and $-2\pi/L$ for $K = -2\pi/L$. With the increase in the strength of the repulsive interaction, the height of the peaks also shrinks and the momentum distributions become broader.

**V. CONCLUSIONS**

In summary, we have exactly solved the problem of two heteronuclear atoms interacting with a short-range $\delta$ potential in a ring trap. For the general case with an arbitrary mass ratio $\alpha$, the relative momentum is coupled with center-of-mass momentum due to the periodic boundary condition. By taking the generalized Bethe-ansatz-type wave function, we have presented a detailed derivation of the analytical solution. While $\alpha = 1$, our solution reduces to the Bethe-ansatz solution of the two-particle Lieb-Liniger model. We have applied our analytical results to studying the energy spectrum, density distribution and momentum distributions of the heteronuclear system, which differ from the case of identical atoms.

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