Self-trapping of Bose-Einstein condensates in optical lattices

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The self-trapping phenomenon of Bose-Einstein condensates (BECs) in optical lattices is studied by numerically solving the Gross-Pitaevskii equation. Our numerical results reproduce the self-trapping that was observed in a recent experiment [Anker *et al.*, Phys. Rev. Lett. **94**, 020403 (2005)]. However, we do not find that the appearance of the steep edges on the boundaries of the wave packet is the critical signal of the selftrapping. More importantly, we discover that the self-trapping breaks down at long evolution times; that is, the self-trapping in optical lattices is only temporary and has a lifetime. This temporariness is caused by the tunneling of atoms at the edge of the BEC wave packet towards outside wells. Our analysis shows that the phenomena observed numerically can all be understood by regarding the optical lattice as a train of doublewell potentials.

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I. INTRODUCTION

Progress in recent years has shown that a Bose-Einstein condensate (BEC) in an optical lattice is a fascinating periodic system, where the physics can be as rich as in fermion periodic systems, the main subject of condensed-matter physics. In such a bosonic system, people have observed well-known and long predicted phenomena, such as Bloch oscillations [1] and the quantum phase transition between superfluid and Mott insulator [2]. More importantly, there are new phenomena that have been either observed or predicted in this system, for example, nonlinear Landau-Zener tunneling between Bloch bands [3,4] and the strongly inhibited transport of one-dimensional BEC in an optical lattice [5].

Another intriguing phenomenon, self-trapping, was recently observed experimentally in this system [6]. In this experiment, a BEC with repulsive interaction was first prepared in a dipole trap. By adiabatically ramping up an optical lattice, the BEC was essentially transformed into a Bloch state at the center of the Brillouin zone. With the optical lattice always on, the BEC was then released into a trap that serves as a one-dimensional waveguide. The evolution of the BEC cloud inside the combined potential was studied by taking absorption images. When the number of atoms in the BEC is small, say around 2000, the BEC wave packet was found to expand continuously (which is expected). However, when the number of atoms was increased to about 5000, it was observed that the BEC cloud stops to expand after initially expanding for about 35 ms (see Fig. 1). This is quite counterintuitive. Even without interaction, a wave packet with a narrow distribution in the Brillouin zone expands continuously inside a periodic potential. When there is an interaction between atoms and it is repulsive, one would certainly expect the wave packet to expand. Moreover, one would expect that the BEC cloud expands faster when the BEC cloud is denser as the result of stronger repulsive force. The experiment showed the contrary: if the cloud is dense enough, it self-traps and stops spreading.

There are now two explanations of this counterintuitive self-trapping phenomenon. The authors of Ref. [6] offered an explanation themselves. They suggested that the self-trapping in the optical lattice is closely related to the self-trapping in a double-well potential [7-10]. The other explanation is proposed in Ref. [11], where a new localized nonlinear wave, gap wave, is found and used to explain the self-trapping. Consequently, there arises a controversy regarding which explanation is right.

To understand this intriguing phenomenon and also as an attempt to resolve the controversy mentioned above, we have carried out an extensive numerical study of this system with the one-dimensional (1D) Gross-Pitaevskii equation. Our results match quite well with the experimental data as shown in Fig. 1. When the atom number N in the BEC is 2000, the agreement between our numerical results and the experiment is excellent; when N=5000, our results are about 40% larger than the experimental data. This discrepancy is likely caused by the higher density: with higher density the lateral motion of the BEC cloud may become more relevant to the longitudinal expansion; however, the lateral motion is completely



FIG. 1. The width of the BEC wave packet as a function of time for N=2000 and N=5000. N is the number of atoms in the BEC. The solid lines are our numerical results while the circles and squares are experimental data from Ref. [6].

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FIG. 2. The width of the BEC wave packet as a function of time for N=2000 (dashed line), 3000 (dotted line), 5000 (solid line), and 50 000 (dashed-dotted line).

ignored in our numerical study as we use the 1D Gross-Pitaevskii equation.

We have analyzed our numerical results in details. Our analysis shows that the expanding dynamics of a BEC cloud in an optical lattice, including the appearance of steep edges and the self-trapping, can be well understood by regarding the optical lattice as a train of double-well potentials. In other words, our study is in support of the explanation in Ref. [6].

However, this support is only partial as our study differs from Ref. [6] on two major features of the BEC cloud expansion. First, we find that the appearance of the steep edges does not always lead to self-trapping as widely believed [6,11]. Second, we discover that the self-trapping is only temporary. After a sufficiently long evolution time, the selftrapping breaks down and the wave packet starts to expand again as seen in Fig. 2. Since the breakdown time is much longer than the observation used in the current experiment [6], these results need to be verified in future experiments. Our numerical analysis shows that the breakdown of selftrapping is caused by the small tunneling of atoms near the edges of the BEC cloud towards outside wells.

If the explanation of the self-trapping as a gap wave in Ref. [11] were true, it would imply that the self-trapping is not temporary, which contradicts with our numerical results. This may indicate that the new gap state has nothing to do with the self-trapping observed in the experiment. More study is certainly needed to clarify the issue.

This paper is organized as follows. In Sec. II, we describe our numerical method and the basic features of the wave packet evolution that we have observed in our numerical simulation. In Sec. III, we offer a detailed analysis of our numerical results in an attempt to understand the appearance of steep edges and self-trapping. In Sec. IV, the lifetime of the self-trapping is discussed. The paper ends with a conclusion section.

II. WAVE PACKET EVOLUTION

To model the experiment, we use the following Gross-Pitaevskii (GP) equation

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t) + V_0\cos(2k_L x)\psi(\mathbf{r},t) + V_{wg}(\mathbf{r})\psi(\mathbf{r},t) + \frac{4\pi\hbar^2 a_s}{m}|\psi(\mathbf{r},t)|^2\psi(\mathbf{r},t), \quad (1)$$

where *m* is the atomic mass, a_s is the *s*-wave scattering length, k_L is the wavelength of the laser that generates the optical lattice, and $V_{wg}(\mathbf{r})$ describes the waveguide potential. Due to the tight confinement perpendicular to the optical lattice from the waveguide potential, the dynamics of this system is largely one dimensional. This allows us to integrate out the two perpendicular directions and reduce the above GP equation to

$$i\frac{\partial\psi(x,t)}{\partial t} = -\frac{1}{2}\nabla^2\psi(x,t) + V\cos(x)\psi(x,t) + \frac{1}{2}\omega x^2\psi(x,t) + g|\psi(x,t)|^2\psi(x,t),$$
(2)

where we have made the equation dimensionless. In doing so, we have x in units of $1/2k_L$ and t in $m/4\hbar k_L^2$. The strength of the optical lattice is given $V=V_0/16E_r$ with $E_r=\hbar^2 k_L^2/2m$ being the recoil energy. For the nonlinear interaction, we have

$$g = \frac{\pi a_s m \omega_\perp N}{\sqrt{2\pi\hbar k_L}},\tag{3}$$

where *N* is the total number of the BEC in the harmonic trap and ω_{\perp} is the transverse trapping frequency of the waveguide. The other frequency ω is so chosen that the initial rms width of BEC wave packet is 7.6 μ m as in the experiment [6]. This width corresponds to about 100 wells occupied. The wave function ψ is normalized to one. In our numerical simulation, we use the following values from the experiment [6], $\lambda = 2\pi/k_L = 783$ nm, $V_0 = 10E_r$, and $\omega_{\perp} = 2\pi \times 230$ Hz.

To simulate the experiment, we prepare our initial wave function ψ to be the ground state in the combined potential of $V \cos(x) + \frac{1}{2}\omega x^2$. This is achieved by integrating Eq. (2) with imaginary time. In the experiment, the waveguide potential also has a longitudinal trapping frequency at $\omega_{\parallel} = 2\pi$ Hz, which is very weak and can be ignored. Therefore, after obtaining the initial wave function, we completely remove the longitudinal trapping and let the wave function evolve according to the following equation:

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\nabla^2\psi + V\cos(x)\psi + g|\psi|^2\psi.$$
 (4)

The evolutions are subsequently recorded and analyzed.

We have computed the evolution of the wave packets for different numbers of atoms in the BEC. As indicated in Eq. (3), the number of atoms in the BEC translates into the non-linear parameter: the larger the atom number N, the stronger the nonlinearity (or the repulsive interaction between atoms). Figure 2 illustrates how the width of a wave packet evolves for different atom numbers.

It is clear from this figure that, when the BEC is dilute and has small atom numbers, $N \leq 2000$, the wave packet expands continuously without stopping as one may have ex-



FIG. 3. Time evolution of the wave packet density for N=2000.

pected. Also as expected, in this range, when the number of atoms increases, the expansion becomes faster. The evolution becomes very different when the BEC is denser. As shown in Fig. 2, for N=3000, the wave packet expansion slows down around 70 ms and becomes slower than that for N=2000 around 85 ms. This means that the expansion is slower for a denser cloud of repulsive interaction, which is counterintuitive. As the cloud gets denser with more atoms, the expansion slows down further. Around N=5000, there even appears a plateau where the cloud stops expanding and becomes self-trapped as observed in the experiment [6]. Figure 2 illustrates a key point: the intriguing self-trapping phenomenon is a gradual process. Before it happens, the wave packet expansion already slows down for high enough densities.

What is more interesting is that, in our numerical simulation, the wave packet continues to expand after pausing for 30-40 ms. For N=5000, the expansion restarts at ~85 ms, just beyond the longest observation time in Ref. [6]. Therefore, this continued expansion awaits for verification in future experiments. Nevertheless, the counterintuitive phenomenon, denser clouds expand slower, persists even after the expansion restarts as we can see in Fig. 2. For contrast, we also computed the case of very large atom number $N=50\ 000$. The wave packet is almost never spread after it expands in a very short initial time. This can be understood as that the self-trapping lasts too long to be observed in our numerical simulations.

To get a clearer picture of the evolution processes, snapshots of the wave packet evolution for N=2000 and N=5000 are presented in Figs. 3 and 4, respectively. In Fig. 3, the wave packet expands with a smooth profile before 80 ms (about the longest experimental observation time in Ref. [6]).



FIG. 4. Time evolution of the wave packet density for N=5000.

However, around 85 ms, the steep edges on both sides of the wave packet begin to appear and grow more and more pronounced as the evolution goes on. The wave packet continued to expand and the steep edges keep moving out during the time evolution. No self-trapping occurs for N=2000.

For the wave packet of N=5000, as shown in Fig. 4, after initial expanding with a smooth profile from t=0 to about 30 ms, steep edges are growing pronounced on both sides of the wave packet. In the subsequent evolution, the wave packet stops expanding out and the positions of the steep edges do not move out any further from t=30 to 80 ms. When compared with the width in Fig. 1, it is clear that this appearance of the steep edges coincides with the nonspreading of the wave packet. Therefore, it is quite natural to believe that the steep edges in Fig. 4 is the signal of the emergence of the self-trapping. However, the case of N=2000 that we considered above indicates otherwise: the steep edges do not always lead to the self-trapping of the wave packet.

We shall next analyze in detail our numerical results, in an attempt to understand these two intriguing phenomena, steep edge and self-trapping.

III. STEEP EDGE AND SELF-TRAPPING

As our discussion goes on, it will become very clear that one can regard the optical lattice as a train of double-well potentials and much of the dynamics of a BEC in the optical lattice can be understood in terms of the dynamics of a BEC in the double-well potential. Therefore, we pause here to give a brief recount of the basic features of the double-well system.

A. Double-well model

For a BEC in a double-well potential, its Hamiltonian can be written as [7,8,10]

$$H_{\text{classical}} = -\frac{c}{2}s^2 + v\sqrt{1-s^2}\cos\theta,$$
 (5)

where *c* is the nonlinear parameter describing the interaction between atoms, and *v* is the coupling constant between the condensates in the two wells. $\theta = \theta_b - \theta_a$ is the relative phase between the two wells *a* and *b* while *s* is the fractional population difference $s = (N_b - N_a)/(N_a + N_b)$ with N_a and N_b being the number of atoms in wells *a* and *b*, respectively. The dynamical equation derived from this Hamiltonian can be expressed as

$$\dot{s} = v \sqrt{1 - s^2} \sin \theta, \tag{6}$$

$$\dot{\theta} = -cs - \frac{vs\cos\theta}{\sqrt{1-s^2}},\tag{7}$$

where \dot{s} is the atom current between these two wells.

It has been known for a while that the self-trapping occurs in this double-well system [7,8,10] and it was observed experimentally [9].

Previous studies [7,8,10] show that there are two types of self-trapping in the double-well system, depending on the ratio $\xi = c/v$ and the population difference *s* in Eq. (5). They are (1) if $1 < \xi < 2$ and the relative phase θ is around π , then the self-trapping occurs when s > 0.5. This is called "oscillation type" self-trapping. (2) If $\xi > 2$ and s > 0.5, another type of self-trapping emerges with the relative phase θ between the two wells increasing with time. Therefore, it is called "running phase type" self-trapping.

B. Steep edges

In Sec. II, we have shown how the density profile of the BEC cloud evolves in time. It is clear from Eqs. (6) and (7) that to fully understand the dynamics we also need to know how the relative phase changes in time. In Figs. 5 and 6, we have plotted how the relative phase between each pair of neighboring wells evolves in time for two typical cases N = 2000 and N = 5000. In our calculation, the relative phase θ is defined as the phase difference between the middle points of the two neighboring wells.

We first focus on Fig. 5 for the case of N=2000. Initially, the relative phase is zero for every pair of double wells in the optical lattice as indicated by a horizontal line. As the evolution goes on, the atoms flow from the wells with high density to outside wells with low density, and the line of relative phase begins to incline with an increasing slope. This increasing slope is an indication that the atoms are moving faster as more interaction energy is converted into the kinetic energy during the wave packet expansion.

Note that the negative value of the relative phase in the figure indicates that the atoms flow to the left while the positive value is the result of the atoms flowing to the right.

The inclination tendency of the line in Fig. 5 stops when the two endpoints of the line reach $\pm \pi/2$, respectively. This



FIG. 5. The evolution of relative phases for each pair of neighboring wells in the optical lattice. N=2000.

is around t=80 ms, right when the steep edges appear. This seems to suggest that the relative phase θ reaching the value of $\pm \pi/2$ at the edges of the BEC cloud is related to the appearance of steep edges. This is indeed the case as we notice from Eq. (6) that the atom current is the largest when $\theta = \pm \pi/2$. More specifically, consider three neighboring wells, *a*, *b*, and *c*. If the relative phase θ_{ab} between wells *a* and *b* is $\pi/2$ and $\theta_{bc} \neq \pi/2$, then there will be more atoms flowing into well *b* than flowing out, leading to the appearance of the steep edges.

As shown in Fig. 6, the situation is similar for N=5000. We also observe that the appearance of steep edges is associated with that the relative phases reach $\pm \pi/2$ near the edges of the wave packets.

We have also computed how the wave packet evolves in the quasimomentum space. To achieve this, we expand the wave packet in terms of the Bloch waves belonging to the lowest Bloch band of the linear system with the periodic potential $\cos x$. The results are shown in Fig. 7, where there is not a large population around k=1/4. Therefore, we do not see the link between the formation of steep edges and the population at k=1/4 as suggested in Ref. [6].



FIG. 6. The evolution of relative phases for each pair of neighboring wells in the optical lattice. N = 5000.

C. Self-trapping in optical lattices

As mentioned in Sec. III A, the self-trapping of a BEC occurs in a double-well potential only under certain conditions. Our following numerical analysis shows that on the one hand, whenever the self-trapping happens in an optical lattice, a few double wells near the edges of the wave packet always satisfy the self-trapping conditions; on the other hand, if no pairs of double well satisfy the self-trapping conditions, then there is no self-trapping in the optical lattice. As a result, we establish a solid link between the self-trapping in the double-well system and the self-trapping in the optical lattice, which was suggested in Ref. [6].

Since the self-trapping condition in the double-well system is given by the ratio $\xi = c/v$ and the population difference *s*, we have computed ξ and *s* for each pair of the neighboring wells in the optical lattice for a given wave packet. The details of how ξ is computed for neighboring wells in an optical lattice can be found in the Appendix.

Figure 8 shows one set of such calculations for a wave packet with N=5000 at t=40 ms, which is the time when the self-trapping happens. It is clear from Fig. 8(a) that there are four pairs of double wells whose ξ and s satisfy the condition for the "running phase type" self-trapping in the double-well system. Furthermore, two of these four pairs, marked by A



FIG. 7. Time evolution of the wave packet in the quasimomentum space for N=5000 with the optical lattice potential V=10 and the rms width of the wave packet 7.6 μ m.

and *B* in Fig. 8, are located right at the two edges of the wave packet. The other two are just nearby; for clarity we do not mark them. This suggests that the self-trapping pairs of neighboring wells around the edges serve as two dams on the both sides of the wave packet, stopping the flow of atoms to the outside. In addition, we have checked the neighboring wells inside the steep edges and find that they do not satisfy the double-well self-trapping condition. For these pairs of double wells, the population difference *s* is smaller than 0.5 although ξ 's are larger than 2.

To further confirm this link, we need to check if there exist the neighboring wells that satisfy the double-well self-trapping conditions for the case of N=2000. Figure 9 shows that the values s and ξ for the wave packet with N=2000 at t=110 ms. This is the time when the steep edges have already developed. We see from the figure that all the values of ξ are smaller than one: the self-trapping conditions of the double-well system are not satisfied by any pair of neighboring wells in the optical lattices.

The above analysis shows that the self-trapping in optical lattices happens only when there exist neighboring wells that satisfy the self-trapping condition of the double-well system. When no pair of the neighboring wells in the lattice satisfies the double-well self-trapping condition, there is no selftrapping in the optical lattice. So established is a solid link



FIG. 8. The values of ξ and s of a wave packet at t=40 ms for N=5000. (a) The values of ξ at different wells. The ξ at the *n*th well is for the double wells composed of the *n*th and (n+1)th wells. (b) Phase diagram (or distribution) of ξ and s for this wave packet. The frame in (b) indicates the self-trapping region.

between these two self-trapping phenomena. One intuitive way of understanding this link is such: Once the selftrapping happens in some pairs of neighboring wells around the edges of a wave packet, these self-trapped double-wells, behaving like "dams," stop the tunneling of atoms towards outside, causing the nonspreading of the wave packet. In Fig.



FIG. 9. The values of ξ and *s* of a wave packet at *t*=110 ms for N=2000. (a) The values of ξ at different wells. The ξ at the *n*th well is for the double wells composed of the *n*th and (*n*+1)th wells. (b) Phase diagram (or distribution) of ξ and *s* for this wave packet. The time 110 ms is when the steep edges start to appear.



FIG. 10. Phase diagrams (or distributions) of *s* and ξ for wave packets at different evolution times. *N*=5000.

10 we have plotted a series of "phase diagrams," where the distribution of the *s*- ξ pairs is shown. The rectangular region in each panel is the area where the self-trapping conditions are satisfied. We can see clearly from this figure that the double-well self-trapping happens from about *t* = 30 ms to 80 ms for *N*=5000, coinciding with the self-trapping in the optical lattice. We have also checked the cases of *N*=7000 and *N*=50 000 and reached the same conclusion.

Based on the link between these two self-trappings, it is also possible to understand why the BEC cloud expands slower around N=3000 than N=2000 shown in Fig. 2. As one can imagine, when the cloud density increases, some pairs of the wells will get close to satisfy these self-trapping conditions and eventually satisfy them. For the medium densities, e.g., N=3000, there should be a few pairs of the wells that satisfy the conditions just barely. As a result, the selftrapping conditions can be easily or quickly destroyed by the "dripping" effect mentioned above. However, as the cloud expands, the self-trapping conditions can again be satisfied by some pairs of wells further inside and then destroyed again. This on-and-off process can dramatically lead to slowing down of the cloud expansion. What is a pity is that this straightforward picture is hard to be corroborated by our numerical computation because the values s and ξ for neighboring wells can only be computed approximately. Alterna-



FIG. 11. Phase diagram of the self-trapping with the optical lattice potential V=10.

tive methods may be needed to verify this picture.

So far, we have studied only the wave packets whose initial width is 7.6 μ m as in the experiment. In general, the self-trapping depends on the initial widths of the wave packets. We have investigated how the initial width influences self-trapping. Shown in Fig. 11 is a phase diagram of self-trapping with respect to the total atom number and the initial width of the wave packet. The figure shows that for a given atom number the initial width must be small enough for the self-trapping to happen. This is understandable since the key in self-trapping is that the interatomic interaction must be strong enough. A wider initial wave packet for a given atom number means weaker interaction.

IV. LIFETIME OF THE SELF-TRAPPING

According to Fig. 2, the width of the wave packet for N= 5000 continues to increase after staying at a certain value from t=30 to 80 ms. This means that the self-trapping does not stay forever. This breakdown of self-trapping is likely caused by the leakage of atoms at the outmost wells, which we call the dripping effect. At the outmost wells, the density of the BEC is very low and the self-trapping conditions of the double-well system can never be satisfied. As a result, the atoms can tunnel towards outside. The amount of atoms tunneling out is very small and has not much effect on the evolution of the whole cloud for a short time. However, for a long evolution time, this small amount of "dripping" can lead to the significant decreasing of atom numbers in the self-trapping wells and thus destroy the self-trapping. This is similar in spirit to that small cracks can cause the collapse of a dam in a long time. The lifetimes of the self-trapping are calculated and shown in Fig. 12. This figure shows that the larger number of the particles, the longer the lifetime for the self-trapping.

As shown in Fig. 2, the turn from the self-trapping to reexpansion is not very sharp, leading to some ambiguity how to calculate the lifetime. We notice that the width of the wave packet has a small bump at the beginning of the selftrapping, followed by a shallow dip. We take the tip of the small bump as the beginning of the self-trapping. The ending point is taken as the point where the wave packet regains its



FIG. 12. Lifetimes of the self-trapping for different particle numbers with the optical lattice potential V=10 and the initial rms width of the wave packet 7.6 μ m.

tip value of the small bump at the tail of the dip.

To learn some detailed knowledge of these "dripping" atoms, we have monitored in Fig. 13 the growth of the atom number in the 110th and 200th wells. At the beginning, there are no atoms in both wells. Then around t_1 =83.9 ms, there is a sudden increase of atom number in the 110th well as the result of the atoms "dripping" out of the inside wells. At a later time t_2 =189.7 ms, we also see a sudden jump of atom number in the 200th well. This tells us that it takes about 1.18 ms for the atom to "drip" from one well to a neighboring well. We estimate that the lowest energy gap in the double-well potential is about 0.077 E_r . Therefore, the tunneling time between the two wells is about 1.8 ms, which agrees very well with 1.18 ms considering how rough our estimation is. This indicates that the "dripping" atoms go from one well to another well by tunneling through the energy barrier.

There is a recent work, which explains the self-trapping in the optical lattice in terms of truncated Bloch waves [11]. It is not very clear how this explanation is related to our explanation in terms of the double-well self-trapping. It seems that if the explanation with truncated Bloch waves is right, then the self-trapping should be permanent. It is in contradiction



FIG. 13. The relative atom number versus time in the 110th (dashed line) and 200th (solid line) wells for N=5000 with the optical lattice potential V=10 and the initial rms width of the wave packet 7.6 μ m.

with our numerical finding that the self-trapping is temporary. More study is certainly needed to clarify the issue.

V. CONCLUSION

With the Gross-Pitaevskii equation, we have studied numerically the wave packet dynamic of a BEC in a onedimensional optical lattice. We have reproduced the selftrapping observed in a recent experiment [6]. More importantly, we have discovered two major features in the wave packet expansion dynamics. First, we find that the appearance of the steep edges does not always lead to selftrapping. Second, the self-trapping is found to have a lifetime; that is, the cloud expansion stops only temporarily. We have analyzed in detail the numerical results and found that the wave expansion dynamics of a BEC in an optical lattice can be well understood by regarding the optical lattice as a train of double-well potentials.

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APPENDIX: COMPUTATION OF ξ IN OPTICAL LATTICES

We choose one well and its neighbor as a double-well trap. The GP equation is as Eq. (4) except the potential is replaced by $V(x)=V\cos(x)$ for $|x|<2\pi$ and V(x)=V for $|x|>2\pi$. Then we write the wave function as a two-mode wave function, $\phi = au_1(x) + bu_2(x)$ and let $|a|^2 = N_a/(N_a + N_b)$ and $|b|^2 = N_b/(N_a + N_b)$ (N_a is the particle number in well a and N_b the particle number in well b). Plugging the double mode wave function into the GP equation with potential V(x) and using the tight-binding approximation, we obtain the effective Hamiltonian

$$H_{\rm eff} = -c/2(|a|^2 - |b|^2)^2 + v(a^*b + ab^*), \qquad (A1)$$

where the parameter $c = (N_a + N_b)N_g \int |u_1(x)|^4 dx$ and $v = N \int \left[-\frac{1}{2} \nabla u_1^*(x) \nabla u_2(x) + V'(x) u_1^*(x) u_2(x) \right] dx$. The wave function $u_1(x)$ [or $u_2(x)$] is obtained as a ground state from Eq. (4) with single well $\tilde{V}(x) = V \cos(x)$ for $0 < x < 2\pi$ and $\tilde{V}(x) = V$ for other x values.

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