Localized States in a Periodic Potential with Harmonic Confinement

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We analyze the one-dimensional problem of a particle placed in periodic potential with additional harmonic trapping within tight-binding approximation. We find the eigenstates localized on the sides of the harmonic trapping potential. We show that the existence of these states leads to the freezing of the dipole oscillation observed in the experiment of Cataliotti et al. *Science* **293**, *843 (2001)*.

topics: periodic potential, localized states

1. Introduction

The study of the ultracold clouds of bosonic atoms placed in the periodic potentials attracted a lot of interest. The main reason is that the parameters of such systems are widely tunable, allowing for the investigation of different and fundamental issues of quantum mechanics, ranging from quantum phase transitions [1], quantum atom optics [2], atom interferometry [3], and dynamics of Bloch oscillation [4].

In experiments, the atoms usually, apart from being in a periodic potential, are trapped in harmonic confinement. In many cases, the harmonic confinement is asymmetric, resulting in a highly elongated cloud, which can be treated as a quasi-one-dimensional system. Such a system was the subject of many theoretical papers [5–9].

In this paper, we focus on the ultracold cloud of bosonic atoms placed in the strongly elongated harmonic cigar-shaped trap with additional periodic potential (created by optical lattice). In such a case, we deal with a system of a one-dimensional array of Josephson junctions [4], in which the use of tight-binding approximation is common.

Such a system was investigated theoretically in [5]. There, the authors considered the motion of Bose–Einstein condensate (BEC) placed in such a potential, where initially the harmonic trap was suddenly displaced by a certain distance. If the displacement was small, the BEC performed periodic oscillations around the trap center. However, for larger displacement, the BEC remains localized on the side of the harmonic trap. The authors of [5] call this effect “classical dynamical superfluid–insulator transition” and attribute it to discrete modulational instability, occurring when the BEC center of mass velocity is larger than a critical value.

A similar situation was seen in the experiment described in [4]. There, a system of a one-dimensional array of Josephson junctions was realized, and the harmonic trap was initially suddenly displaced. If the above happened with BEC, it performed dipole oscillation. On the other hand, when the trapped gas was a thermal cloud, its center of mass remained localized on the side of the harmonic trap. The authors of [4] attributed this phenomenon to the lack of an overall macroscopic phase.

In the present paper, we investigate theoretically the system of a one-dimensional array of Josephson junctions. We analyze the single-particle problem and find states localized at the borders of the harmonic potential, which show a void of single-particle probability in the center of the trap. We show how the existence of such states explains the phenomena in both of the above-mentioned papers.

In Sect. 2, we analyze the solution of the tight-binding approximation model, showing the existence of eigenstates localized on the sides of the harmonic trap. In Sect. 3, we use semiclassical approximation to analyze those eigenstates. In Sect. 4, we discuss the results of the experiment described in [4], showing that the phenomena observed in this experiment can be attributed to the existence of localized states. We finish with a short summary of the results.

2. Theoretical model

We begin with an analysis of a noninteracting system placed in periodic potential with additional harmonic confinement

$$V(\boldsymbol{r}) = \frac{1}{2} m\left[\omega_r^2(x^2+y^2) + \omega_z^2 z^2\right] + V_0 \sin^2\left(2\pi\frac{z}{\lambda}\right), \quad (1)$$

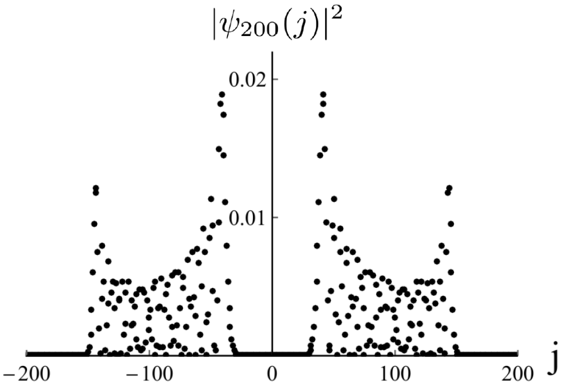

Fig. 1. Density $|\psi_{200}(j)|^2$ for $\Omega/J \simeq 1/5000$ as the function of well number j (given by integer number). Here, $\psi_{200}(j)$ is the numerical solution of (5). As $\sum_j |\psi_{200}(j)|^2 = 1$, the values of $|\psi_{200}(j)|^2$ are dimensionless real numbers (given on the vertical axis). We clearly see that the presented eigenstate density vanishes in the center of the trap — the state is localized at the borders.

where m is the atomic mass, and ω_r and ω_z are frequencies of the harmonic trapping potential in the x–y direction and z direction, respectively. In addition, we notice potential generated by the optical lattice with a maximal value equal to V_0 and λ denoting the wavelength of the laser light producing the lattice. We assume that the excitation energy of the system is always smaller than $\frac{1}{2}\hbar\omega_r$, and the system stays in the ground state for x and y directions.

The single-particle Schrödinger equation takes the standard form

$$\mathrm{i}\hbar\,\partial_t\psi(\boldsymbol{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right)\psi(\boldsymbol{r},t). \tag{2}$$

If V_0 is large enough, the wave function remains localized in the wells of the periodic potential, and the movement between the neighboring wells is due to the tunneling process. Then, the system can be described within tight-binding approximation, where the wave function is represented as

$$\psi(\boldsymbol{r},t) = \sum_j \psi(j,t)\,\Phi(z-j\lambda)\,\phi_0(x)\phi_0(y), \tag{3}$$

where $\psi(j,t)$ is the j-th site amplitude and $\Phi(z)$ is the Wannier function connected with the lattice potential. In the above, the function ϕ_0 is the ground state of the one-dimensional harmonic oscillator of frequency ω_r. Upon substituting (3) into (2), we obtain

$$\mathrm{i}\hbar\,\partial_t\psi(j,t) = -J\big(\psi(j{+}1,t) + \psi(j{-}1,t) - 2\psi(j,t)\big) + \Omega j^2\psi(j,t), \tag{4}$$

where $J = \frac{\hbar^2}{2m}\int \mathrm{d}z\ \Phi(z)\partial_z^2\Phi(z-\lambda)$ is the tunneling coefficient, and $\Omega = \frac{1}{2}m\omega_z^2\lambda^2$. Note that j denotes the well number and is given by the integer number.

In the stationary case $\psi(j,t) = \mathrm{e}^{-\mathrm{i}E_n t/\hbar}\psi_n(j)$ and upon substituting it into (4), we arrive at

$$E_n\psi_n(j) = -J(\psi_n(j+1) + \psi_n(j-1) - 2\psi_n(j)) + \Omega j^2\psi_n(j). \tag{5}$$

From the above, we clearly see that the solution $\psi_n(j)$ depends on a dimensionless parameter Ω/J with the energy E_n/J. Solving numerically the above equation for $\Omega/J \ll 1$, one finds two kinds of states: low-lying states, which resemble the harmonic oscillator eigenstates, and higher states, for which single-particle probability density is localized on the borders of the trap. In Fig. 1, we present $|\psi_n(j)|^2$ for $n = 200$, where $\psi_n(j)$ is defined as a solution of (5). We choose $\Omega/J \simeq 1/5000$. The horizontal axis give, the well number j — an integer number. The state is normalized to unity, i.e., $\sum_j |\psi_{200}(j)|^2 = 1$, and from this condition, we find $|\psi_{200}(j)|^2$ is a dimensionless number.

We clearly see that the density vanishes in the center of the trap, which indicates that the state is localized at the borders.

3. Semiclassical analysis

To understand, in simple terms, the existence of such a solution, we move to the semiclassical analysis of (4) and (5). Equation (4) in momentum space takes the form

$$\mathrm{i}\hbar\,\partial_t\psi(k,t) = \Big[-\Omega\partial_k^2 + 2J(1-\cos(k))\Big]\psi(k,t), \tag{6}$$

where

$$\psi(j,t) = \int_{-\pi}^{\pi} \mathrm{d}k\ \mathrm{e}^{\mathrm{i}kj}\psi(k,t) \tag{7}$$

together with $\psi(k=-\pi,t) = \psi(k=\pi,t)$, $\partial_k\psi(k=-\pi,t) = \partial_k\psi(k=\pi,t)$. As written above, j is the well number given by the dimensionless integer numbers. Therefore, k is given by the dimensionless real number. Due to the above mapping, k is restricted to the range $-\pi \le k \le \pi$. Given the above, we find the analog of Ehrenfest theorem for the mean values of "position" $\langle k\rangle = \int \mathrm{d}k\ k|\psi(k,t)|^2$ and "momentum" $\langle j\rangle = \langle -\mathrm{i}\,\partial_k\rangle$, obtaining

$$\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle k\rangle = 2\Omega\langle j\rangle, \qquad \hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle j\rangle = \langle -\partial_k\widetilde{V}(k)\rangle, \tag{8}$$

where $\widetilde{V}(k) = 2J(1-\cos(k))$. We now assume that the width of the wave-packet $\psi(k,t)$ is much smaller than unity (note that k is defined in the range $-\pi \le k \le \pi$ and is a real dimensionless number). This restriction means that the wave packet in the position space $\psi(j,t)$ (here j denotes the well number given by integer dimensionless numbers) changes on the length of many wells — the length j_{change}, on which $\psi(j,t)$ changes, is much larger than unity. The above assumption makes us approximate $\langle\partial_k\widetilde{V}(k)\rangle \simeq \partial_{\langle k\rangle}\widetilde{V}\,(\langle k\rangle)$. As a result, we obtain the classical equation of motion for the mean values of "position" $k = \langle k \rangle$ and "momentum" $j = \langle j \rangle$

$$\hbar \dot{k} = 2\Omega j, \quad \hbar \dot{j} = -\partial_k \widetilde{V}(k) = -2J\sin(k) \tag{9}$$

with the Hamiltonian given by

$$\hbar H = \Omega j^2 + \widetilde{V}(k) = \Omega j^2 + 2J\big(1-\cos(k)\big). \tag{10}$$

We now proceed with the analysis based on the above semiclassical Hamiltonian. We can see that this is a Hamiltonian of a pendulum in a gravitational field with kinetic energy term Ωj^2 and potential energy term $2K(1-\cos(k))$. For $k \ll 1$, we can approximate the potential energy term by Jk^2. As a result, we obtain a harmonic oscillator Hamiltonian. This happens for energies of the system much smaller than J. For higher energies, we notice increasing anharmonicity of the movement up to a critical energy equal to $4J$, which is the maximal potential energy of the system. For energies higher than $4J$, the absolute value of the momentum is always larger than zero and bounded by $j_{\max} = \sqrt{E/\Omega} \geq |j| \geq \sqrt{(E-4J)/\Omega} = j_{\min}$. Here, we take energy E equal to $\hbar H$. Referring to the definitions of the momentum j, we see that it means that the physical particle cannot reach the trap center — it moves on the left or right-hand side of the trap between the bounds $\pm j_{\max}$ and $\pm j_{\min}$. The probability distribution $\rho(j)$ to observe the particle in a certain position takes the form

$$\rho(j) = C\, \frac{1}{\sqrt{\left(1-\frac{E}{4J}+\frac{\Omega}{4J}j^2\right)\left(\frac{E}{4J}-\frac{\Omega}{4J}j^2\right)}}, \tag{11}$$

where

$$C = \frac{\sqrt{\Omega/J}}{4\Big[K\left(\frac{E}{4J}\right) + \mathrm{i}K\left(1-\frac{E}{4J}\right)\Big]} \tag{12}$$

is the normalization factor. In the above, K denotes the elliptic integral.

In Fig. 2, we plot $|\psi_{200}(j)|^2$, where $\psi_{200}(j)$ is the solution of the eigenproblem given by (5) for $\Omega/J = 1/5000$ together with the semiclassical probability distribution $\rho(j)$ given by (11) where we take energy E equal to E_{200} obtained from the quantum model. The discrete points of $|\psi_{220}(j)|^2$ are joined by the meshed continuous curve to guide the eye.

We notice good agreement between the averaged (over fringes) quantum density and its semiclassical counterpart.

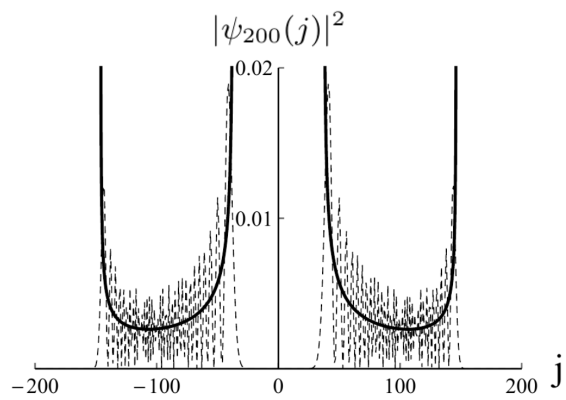

Fig. 2. Density $|\psi_{200}(j)|^2$ for $\Omega/J \simeq 1/5000$ as the function of well number j. Here, we present the same plot as in Fig. 1, but instead of points showing the value of the density $|\psi_{200}(j)|^2$ for discrete values of well number j (given by integer numbers), we show the meshed continuous curve to guide the eye. In addition, we plot the density $\rho(j)$ given by (11) with energy E being equal to E_{200} and given by the solution of (5). We notice good agreement between the averaged (over fringes) quantum density and its semiclassical counterpart.

4. Large thermal cloud movement — experiment by Cataliotti et al. [4]

Here we want to show the consequence of the existence of the above-described localized states. In many experiments performed with ultracold clouds trapped in harmonic potential, the so-called dipole oscillations are investigated. Cloud is displaced by a certain distance from the trap center. If the harmonic trapping potential is the only external potential, then the center of mass of the cloud undergoes harmonic oscillation with a frequency equal to the trapping frequency. It is interesting to note what such movement looks like in the presence of periodic potential. Looking at the semiclassical calculation presented above, it is easy to find out.

We assume that the cloud is dilute enough that we can neglect the interaction between atoms. Additionally, we assume that the tight-binding approximation can be applied. If the size of the cloud (given in lattice sides) added to initial displacement is smaller than j_{crit} defined as $\Omega j_{\mathrm{crit}}^2 = 4J$, then the cloud will perform dipole oscillation with the frequency $2\sqrt{\Omega J}/\hbar$. This is due to the fact that all particles populate the eigenstates that are similar to harmonic oscillator states.

Now, we choose a different case, namely cloud, whose size is significantly larger than j_{crit}. Then, after displacement, a significant part of the cloud particles will populate the above-described localized states. In such a case, those particles will stay localized on the initial side of the harmonic trap. As a result, no dipole oscillation will be observed.

Such a situation was observed experimentally in [4]. There, an ultracold ^{87}Rb gas was placed in an elongated harmonic trap with additional periodic potential

$$V(\boldsymbol{r}) = \frac{1}{2}m\left[\omega_r^2(x^2+y^2) + \omega_z^2 z^2\right] + V_0 \sin^2\left(2\pi\frac{z}{\lambda}\right), \tag{13}$$

where $\omega_r = 2\pi\times 92$ Hz, $\omega_z = 2\pi\times 9$ Hz, $\lambda = 795$ nm, and $V_0 = 3E_R$, where $E_R = \frac{\hbar^2 k^2}{2m}$, $k = \frac{2\pi}{\lambda}$. In this experiment, a thermal cloud of temperature

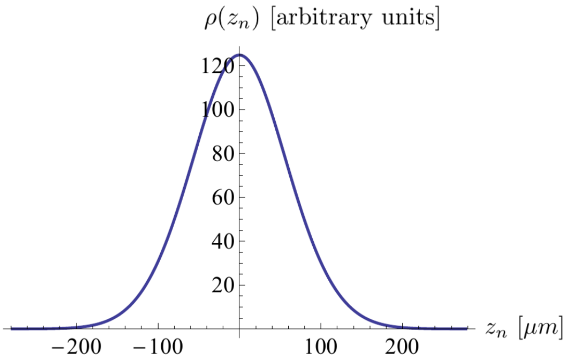

Fig. 3. Single-particle density $\rho(z_n)$ plotted in arbitrary units as a function of position of the n-th potential well, i.e., $z_n = n\frac{\lambda}{2}$, where n is the integer number (please find a detailed description of the plot in the main text). The horizontal axis marks z_n given in micrometers. The discrete points $\rho(z_n)$ are connected with the continuous curve to guide the eye.

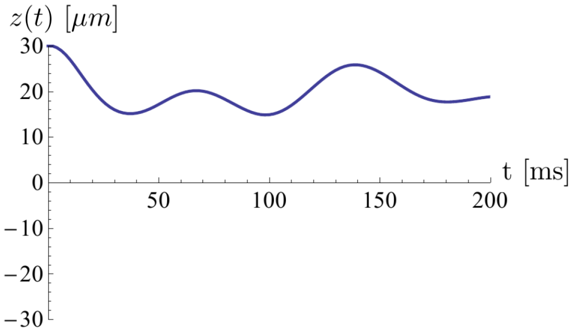

Fig. 4. Temporal thermal cloud mean position evolution $z(t)$ (in micrometers) as a function of time (given in milliseconds).

$T = 130$ nK, slightly above the transition temperature, was prepared [10]. Then, the harmonic trapping potential was suddenly displaced by 30 μm. The cloud started to move, and its center of mass was measured as a function of time. No dipole oscillations were observed — the center of mass stayed on the same side of the harmonic trap. On the other hand, when the periodic potential was turned off (the harmonic trap was still present), the thermal cloud underwent dipole oscillation as expected.

Below, we show that we can attribute the lack of dipole oscillation to the existence of the localized states. We do it without using tight-binding approximation and solve directly the stationary Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\triangle + V(\boldsymbol{r})\right)\psi_n(\boldsymbol{r}) = E_n\psi_n(\boldsymbol{r}). \tag{14}$$

The solution is $\psi_n(\boldsymbol{r}) = \varphi_{nx}(x)\varphi_{ny}(y)\psi_{nz}(z)$ and $E_n = E_{nx,ny,nz} = \hbar\omega_r(1 + nx + ny) + E_{nz}$. In the above, φ_n is the eigenstate of the harmonic oscillator of frequency ω_r, and $\psi_n(z)$ is a solution of

$$\left(-\frac{\hbar^2}{2m}\triangle_z + V_z(z)\right)\psi_{nz}(z) = E_{nz}\,\psi_n(z), \tag{15}$$

where $\triangle_z = \partial^2/\partial z^2$, $V_z(z){=}\frac{1}{2}m\omega_z^2 z^2{+}V_0\sin^2(2\pi\frac{z}{\lambda})$. The initial single-particle density reads

$$\rho(\boldsymbol{r}) = \sum_n n_n|\psi_n(\boldsymbol{r})|^2, \tag{16}$$

where $n_n = \left[\exp(\frac{E_n-\mu}{k_BT}) - 1\right]^{-1}$. The chemical potential μ is found from normalization condition $N = \sum_n n_n = 2\times 10^5$.

To obtain the density of the thermal cloud, we numerically diagonalize (15). From the normalization condition, we find $\exp(-\mu/(k_BT)) \simeq 1.6$. Having this, we may obtain the initial density $\rho(\boldsymbol{r})$ given by (16). In the system, we have lattice periodic potential that gives us well-defined wells. As we shall see, we have about 200 wells occupied by atoms. Thus, looking at the density integrated over x and y, $\rho(z) = \int \mathrm{d}x\mathrm{d}y\ \rho(\boldsymbol{r})$, we would see strong density oscillation connected with the periodic potential. The strength of the amplitude of the oscillation is connected with the harmonic trapping in the z-direction. To make the density plot readable, we plot only the amplitude of density oscillation (forgetting the oscillation part). In order to do so, we show the values of the density $\rho(z_n)$ in the minima of the periodic potential, i.e., $z_n = n\frac{\lambda}{2}$, where n is the integer number. In Fig. 3, we plot the density profile $\rho(z_n)$, connecting the point z_n with the continuous curve to make the plot readable.

At the beginning of the evolution, the potential is suddenly displaced by $z_0 = 30\ \mu m$. For simplicity of the calculation, we displace the thermal cloud so that the single-particle density takes the form

$$\rho(\boldsymbol{r}, t=0) = \sum_n n_n|\psi_n(\boldsymbol{r} - z_0\boldsymbol{e}_z)|^2. \tag{17}$$

As the potential is harmonic and the displacement is along z-axis, φ_{nx} and φ_{ny} do not change during the time evolution while the evolution of $\psi_{nz}(z,t)$ is given by the Schrödinger equation

$$\mathrm{i}\hbar\,\partial_t\psi_{nz}(z,t) = \left(-\frac{\hbar^2}{2m}\triangle_z + V_z(z)\right)\psi_{nz}(z,t), \tag{18}$$

with the initial condition $\psi_{nz}(z,0) = \psi_{nz}(z - z_0)$. To simplify the analysis, we integrate the particle density along x- and y-directions, obtaining

$$\rho(z,t) = \sum_{nz} n_{nz}\left|\psi_{nz}(z,t)\right|^2 \tag{19}$$

where $n_{nz} = \sum_{nx,ny} n_{nx,ny,nz}$. The mean position is given by

$$z(t) = \sum_{nz} n_{nz}\int \mathrm{d}z\ z|\psi_{nz}(z,t)|^2. \tag{20}$$

We now evolve all $\psi_{nz}(z,t)$ using (18) and numerically calculate $z(t)$. The result is shown in Fig. 4. We notice a lack of oscillation, which is in agreement with the experimental results presented in [4].

Now we would like to refer the above results to the one given by the tight-binding approximation

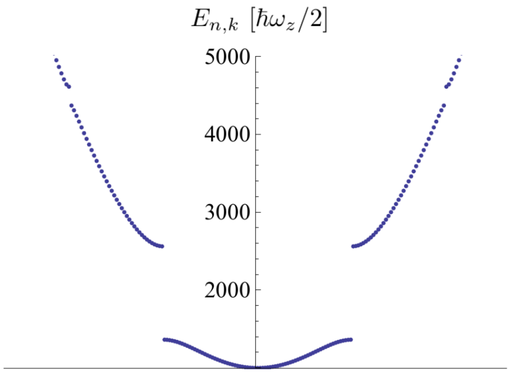

Fig. 5. Energy spectrum $E_{n,k}$ given by the solution of (21). The energy is given in the units of $\hbar\omega_z/2$. On the horizontal axis we have the wavevector k in arbitrary units — the plot is only to show the large energy gap between the first and second energy bands.

model. To do this, we first find the energy spectrum of purely periodic problem solving the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}z^2}+V_0\sin^2\left(2\pi\frac{z}{\lambda}\right)\right]\psi_{n,k}(z)=E_{n,k}\,\psi_{n,k}(z). \tag{21}$$

It is known that the energy spectrum of the periodic potential has a band structure. Above, n denotes the band number, whereas k gives the wavevector in the given band. In Fig. 5, we plot $E_{n,k}$, which is the numerical solution of the above equation in the units of $\frac{1}{2}\hbar\omega_z$. On the horizontal axis we have the wavevector k in arbitrary units — the plot is only to show the large energy gap between the first and second energy bands. It is known that the tight-binding approximation uses only the first band. Therefore, it is reasonable to use this approximation only if the crucial physics refers to the first band; the excited bands can be neglected.

In Fig. 5, we clearly notice the first band with a large gap roughly equal to $\Delta E = 1500\frac{\hbar\omega_z}{2}$. If we define z_b through equation $\frac{1}{2}m\omega_z^2 z_b^2 = \Delta E$, we find $z_b \simeq 196$ μm. Now, if most of the atoms of the cloud are located in region $-z_b < z < z_b$, the tight-binding approximation can be used to correctly describe the system. Looking at Fig. 3, we find that the extent of the thermal cloud is roughly equal to 200 μm. It means that even after displacement by 30 μm, it is reasonable to use tight-binding approximation as an approximate description of the system. When using the tight-binding approximation results described previously, we find that a large fraction of particles populate the localized states. The particles in these states will not perform periodic motion. Only the small fraction of particles that populate the harmonic oscillator states undergoes periodic motion. The sum of both these motions explains the overall lack of periodic motion seen in Fig. 4.

5. Conclusions

In this paper, we have studied the system of noninteracting atoms placed in periodic potential with additional harmonic trapping, using tight-binding approximation. Within numerical analysis, we found eigenstates localized on the sides of the harmonic trap. We explained the properties of these states using semiclassical approximation. Further on, we analyzed the results of the experiment described in [4], in which the large thermal cloud placed in periodic potential with additional harmonic trapping was suddenly displaced from the trap center. The measured center of mass of the cloud showed a lack of periodic motion, present for small condensate cloud. Using the noninteracting atoms model, we observed the same phenomena. Furthermore, we showed that the lack of periodic motion can be attributed to the existence of the localized states mentioned above.

Acknowledgments

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