Quantum localization and bound-state formation in Bose-Einstein condensates

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We discuss the possibility of exponential quantum localization in systems of ultracold bosonic atoms with repulsive interactions in open optical lattices without disorder. We show that exponential localization occurs in the maximally excited state of the lowest energy band. We establish the conditions under which the presence of the upper energy bands can be neglected, determine the successive stages and the quantum phase boundaries at which localization occurs, and discuss schemes to detect it experimentally by visibility measurements. The discussed mechanism is a particular type of quantum localization that is intuitively understood in terms of the interplay between nonlinearity and a bounded energy spectrum.

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I. INTRODUCTION

The phenomenon of Anderson localization in disordered quantum systems [1] was originally discovered in the context of the study of electrons in a crystal with imperfections [2]. In fact, it is much more general [3] and has been observed in a variety of systems, including light waves in random media [4,5]. Despite remarkable efforts, Anderson localization has not been observed directly in crystals, owing to the high electron-electron and electron-phonon interactions. It has finally been observed in noninteracting Bose-Einstein condensates in one-dimensional quasiperiodic optical lattices [6], which feature a crossover between extended and exponentially localized states, as in the case of purely random disorder in higher dimensions; moreover, the effects of random disorder in optical lattices can also be simulated by manipulating the interactions in multispecies mixtures [7]. These achievements are due to the unprecedented degree of control over the system physical parameters, in particular the vanishing of the interaction strength, that ultracold atoms offer.

Indeed, ultracold degenerate gases in optical lattices provide an unprecedented toolbox for the experimental realization of what were once just toy models sketching the key features of complex condensed matter systems. One prominent example is the Bose-Hubbard model [8,9], which was originally introduced as a variant of the better-known Hubbard model and whose properties were later discussed at length in the context of the description of superfluid ^{4}He trapped in porous media. The suggested realization in optical lattices loaded with ultracold bosonic atoms [10] was soon achieved in a spectacular breakthrough experiment [11]. Driven by this brilliant result, a growing number of investigations have focused on the possibility of using optical lattices to realize various phenomena of considerable interest in condensed matter physics [12,13]. Among these, in the last years much attention has been devoted to the study of localized quantum phases in many-body systems. For instance, it has been shown that it is possible to use boundary dissipation [14] or the control of the sign of the local interactions, exploiting Feshbach resonances, to switch from the repulsive Hubbard model to the attractive one, whose ground state may feature a collapse of all the atoms of the system into a single site of the lattice [15–17]. The transition to collapse is essentially due to the combination of the nonlinear dependence of the local Hamiltonian on the site occupation, which makes energetically favorable those states that are characterized by a concentration of all atoms in a single site.

In the present work we describe a route to quantum localization in many-boson systems with repulsive interactions that has one important feature in common with the transition to collapse discussed in Refs. [15–17]. The basic idea is to consider the maximally excited state in the lowest energy band of an interacting system in a nontranslationally invariant lattice. Within the Bose-Hubbard framework this is just the eigenstate with highest energy of a Hamiltonian H with repulsive interactions. This state is then the eigenstate with lowest energy (i.e., the ground state) of a new Hamiltonian H' equal to minus the original Hamiltonian: $H' = -H$. The rotated Hamiltonian has attractive interactions (instead of repulsive interactions) and a negative tunneling amplitude. However, this can be turned positive again by a π-phase shift on every other lattice site. If one can show the occurrence of exponential localization in the highest excited state of the repulsive Hamiltonian, this phenomenon is then completely equivalent to the collapse in the ground state of the corresponding attractive model. In the latter case, upon increasing the intensity of the attraction, the particles form a bound state with increasing mass, which appears to be localized if the correlation length becomes smaller than the lattice spacing. The two mechanisms differ in that the former is not realized as an on-site collapse in the ground state of a system with attractive interactions, but rather as a proper exponential localization in the maximally excited state of the lowest energy band in systems with repulsive interactions. It is thus a mechanism that is solely due to the interplay between nonlinearity and an energy spectrum bounded from above. The latter in turn is a fundamental feature associated with the fact that the Bose-Hubbard Hamiltonian preserves the total particle number.

In the following we will investigate the properties of the maximally excited state of the one-dimensional repulsive Bose-Hubbard model defined on open lattice chains. Such

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analysis, besides resorting to exact diagonalization for systems of very small size, will be carried out for larger systems using numerical solutions obtained with a controllable recursive algorithm as well as a semiclassical approach when the size of the problem makes the numerical computation impractical. We will show that, depending on the physical parameters of the system, the maximally excited state of the repulsive Bose-Hubbard Hamiltonian defined on an open chain features three different phases of which the first one, associated to small values of the local repulsion, is characterized by a relative atomic population spread on all sites of the lattice. At intermediate values of the on-site interaction there occurs a second phase in which a macroscopic fraction of the atoms begins to localize in a single site while the remainder of the atomic population is still spread over the lattice. Finally, we will show that for large values of the on-site repulsion the maximally excited state is characterized by an exponential localization in the center of the lattice, and we will investigate the decay rate both numerically and analytically. We will then determine the physical conditions such that the overlap of the maximally excited state of the lowest energy band with the lowest states of the upper bands can be neglected, and we will discuss how to detect experimentally the three different behaviors by measurements of the visibility.

II. MODEL AND METHODS

Let us consider a system of N ultracold atoms with repulsive on-site interactions described by a Bose-Hubbard model on a one-dimensional lattice of M sites:

$$H = \frac{U}{2} \sum_{j=-d}^{d} \hat{n}_j(\hat{n}_j - 1) - T \sum_{j=-d}^{d-1} (\hat{a}_j^\dagger \hat{a}_{j+1} + \text{H.c.}). \quad (1)$$

One needs to consider open chains to look, even in principle, for the possibility of true localization. Indeed, in a translationally invariant geometry the atoms would be unable to localize on a definite site. Namely, even in the presence of strong repulsive on-site interactions, the maximally excited state would be essentially a Schrödinger-cat state, i.e., a superposition of localized states characterized by a flat distribution of the atomic density over the entire lattice [17]. In Eq. (1) $d = (M - 1)/2$, $\hat{a}_j$ ($\hat{a}_j^\dagger$) are the bosonic annihilation (creation) operators on the jth site, $\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j$ are the occupation number operators, $U > 0$ is the strength of the repulsive nonlinear on-site interaction, and T is the hopping amplitude between neighboring sites.

In order to determine an optimized analytic approximation to the maximally excited state of the Hamiltonian (1) on a finite open chain we proceed by a dynamical variational method and compare results with those obtained by exact diagonalization. We follow the route adopted for the corresponding attractive model [16,17], introducing a macroscopic trial state of the form $|\tilde{\phi}\rangle = e^{i\varphi}|\phi\rangle$, where φ is a time-dependent phase and $|\phi\rangle$ is a coherent state of the form

$$|\phi\rangle = \frac{1}{\sqrt{N!}} \left(\sum_{j=-d}^{d} \phi_j \hat{a}_j^\dagger \right)^N |\Omega\rangle. \quad (2)$$

Here $|\Omega\rangle$ is the vacuum state and the coherent-state constants, $\phi_j \in \mathbb{C}$ for $j = 1, \ldots, M$, must satisfy the normalization condition $\sum_{j=1}^{M} |\phi_j|^2 = 1$. The complex quantities ϕ_j describe the on-site bosonic states by the on-site population $|\phi_j|^2$ and the macroscopic local phase $\arg \phi_j$. The request that the trial state satisfies the Schrödinger equation on the average, $\langle \tilde{\phi} | i \partial_t - H | \tilde{\phi} \rangle = 0$, identifies the time derivative $\dot{\varphi}$ with an effective Lagrangian for the dynamical variables ϕ_j and the corresponding effective Hamiltonian [18]:

$$\mathcal{H} = \frac{U}{2} N(N-1) \sum_{j=-d}^{d} |\phi_j|^4 - TN \sum_{j=d}^{d-1} (\phi_j^* \phi_{j+1} + \text{c.c.}). \quad (3)$$

Maximizing the latter with respect to the variables ϕ_j under the normalization constraint, one obtains a semiclassical variational approximation to the maximally excited energy eigenstate of the system. The first term of Eq. (3), i.e., the on-site interaction term, does not depend on the phases of the on-site variables ϕ_j, while the hopping term, at arbitrarily fixed values of $|\phi_j|$ and $|\phi_{j+1}|$, is maximized by a phase difference $\pm \pi$. Therefore, except for an irrelevant global phase factor, the values ϕ_j associated to the maximally excited state can be assumed to be real quantities with alternating signs. By defining $x_j = |\phi_j|$, and taking into account the property of invariance under mirror reflection ($x_j = x_{-j}$) with respect to the center of the finite chain, Eq. (3) can be recast in the equivalent forms

$$\frac{\mathcal{H}}{N} = \frac{U}{2}(N-1)\left(x_0^4 + 2\sum_{j=1}^{d} x_j^4 \right) + 2T \sum_{j=1}^{d} x_j x_{j-1},$$

$$\mathcal{H} = \Lambda \left(x_0^4 + 2\sum_{j=1}^{d} x_j^4 \right) + \sum_{j=1}^{d} x_j x_{j-1}. \quad (4)$$

Introducing the dimensionless ratio of the interaction to kinetic energy scales, $\Lambda = U(N-1)/(8T)$, one can solve the problem for different values of Λ and maximize Eq. (4) using the hyperspherical representation of the variables x_j to enforce automatically their exact normalization and can then compare the atomic distribution densities so obtained with those provided by exact diagonalization for small samples. The latter in turn can be performed very efficiently with the help of augmented recursive Lanczos algorithms [19]. The result of this comparison is reported in Fig. 1.

Figure 1 shows that the semiclassical solution provides an excellent approximation to the maximally excited state that becomes more and more accurate with increasing strength of the interaction and of the localization of the atoms at the center of the lattice and can thus be extended to systems of much larger size that cannot be investigated by exact diagonalization. More important, Fig. 1 shows that as the Λ parameter varies the atomic density profile in the maximally excited state crosses three different phases. The first one, associated with small values of Λ, is characterized by the absence of localization; the third one, associated with very large values of Λ, corresponds to a complete concentration of all the atoms of the system in the center of the lattice; finally, the second one, associated with intermediate values of Λ, corresponds to the onset of the localization of a significant fraction of the atomic population
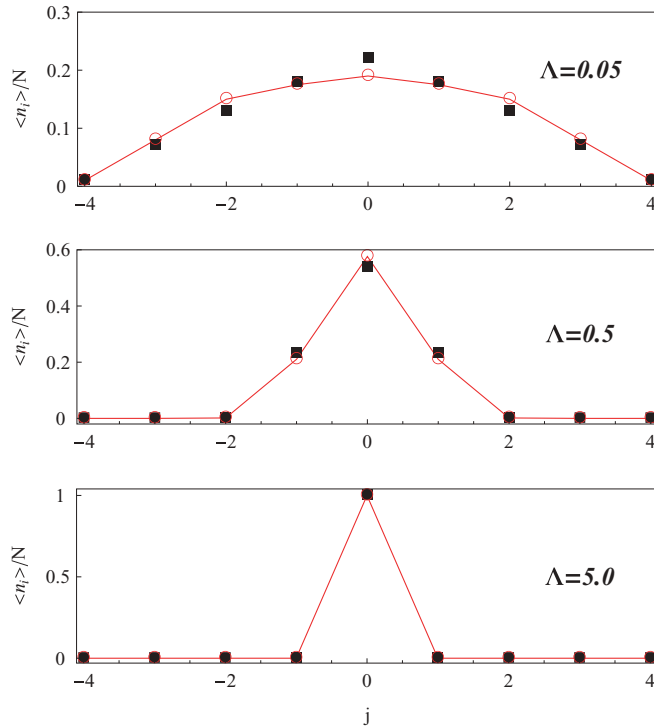
FIG. 1. (Color online) The atomic density profile $\langle n_j \rangle / N$ in the maximally excited state of Hamiltonian (1) obtained by exact diagonalization (full black squares) and by the semiclassical variational approximation (empty circles linked by the solid line) for different values of the dimensionless energy ratio Λ in an open chain of $M = 9$ sites and $N = 9$ atoms. All quantities plotted are dimensionless.

in the central site, while the distribution of the remainder of the atomic population over the entire lattice stays finite.

III. EXPONENTIAL LOCALIZATION AND VISIBILITY

We now investigate in detail the exponential nature of the localization in the maximally excited state. The presence of an exponential decay is reported (on a logarithmic scale) in Fig. 2. It shows the behavior of the relative occupation $\langle n_i \rangle / N$ as a function of the distance from the center of the lattice. The occurrence of an exponential localization allows us to introduce a simple and effective method to obtain an excellent analytical approximate solution to the problem of the maximization of the effective Hamiltonian. We introduce a dimensionless parameter χ and assume $|\phi_j| = \chi^j \; \forall \, j \in [1,d]$, with $|\phi_0| = 1 - 2\chi^2(1 - \chi^{2d})/(1 - \chi^2)$ in order to satisfy normalization. Within this setting the maximization of the effective variational Hamiltonian can be performed analytically. Exploiting the condition $\chi \ll 1$, necessary to have a state localized in the central site, one finds the approximate analytical solution $\chi = \Lambda/8$.

It is worth observing that the expression for χ that determines the approximate solution to the maximally excited state of the system does not depend on the size of the chain. On the other hand, it depends on the number of atoms in the lattice through Λ. In Fig. 3 we have compared the exact numerical solution of the variational problem with the approximate analytical solution for different value of Λ within
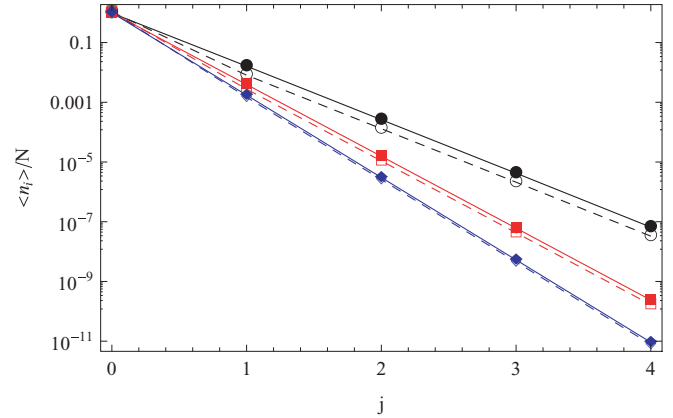

FIG. 2. (Color online) Atomic density distribution (on a logarithmic scale) associated with the maximally excited energy eigenstate in the localized phase obtained by exact diagonalization (solid lines and full symbols) and by the semiclassical variational approximation (dashed lines and empty symbols) for a chain of $M = 9$ sites and $N = 9$ atoms. From top to bottom: circles and lines ($\Lambda = 1.0$); squares and lines ($\Lambda = 2.0$); diamonds and lines ($\Lambda = 3.0$). All quantities plotted are dimensionless.

the interval compatible with localization. One sees that even at moderate values of Λ the analytical approximation reproduces the essential features of the exact localized quantum solution.

The onset of localization in the maximally excited state can be naturally captured either by analyzing the behavior of the relative occupation of the central site $\langle n_0 \rangle / N$ or by looking at the factor $f_0 = 1 - \langle n_0 \rangle / N$ that measures the relative atomic population outside the central site. The upper panel of Fig. 4 shows that for small values of Λ the ratio f_0 is enhanced. In this regime and for very long chains, such that the border effects can be neglected, $f_0 \to 1 - 1/M$. The ratio begins to decrease at the onset of localization at the critical value $\Lambda_c \simeq 0.7$, finally vanishing asymptotically in the limit $\Lambda \to \infty$.
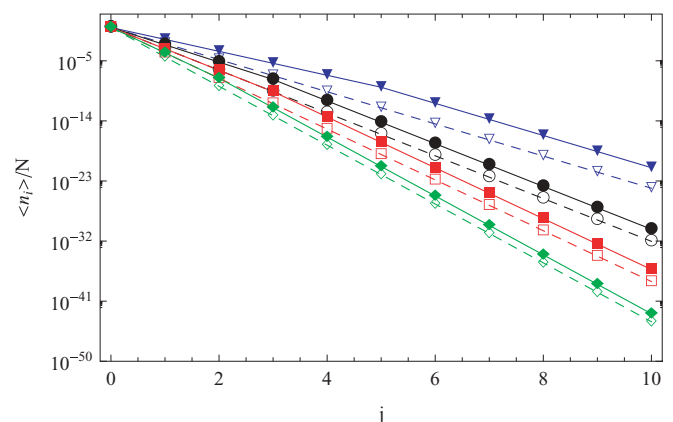

FIG. 3. (Color online) Atomic density distribution (on a logarithmic scale) as a function of the distance from the center of the lattice for an open chain of $M = 21$ sites and $N = 21$ atoms. Solid lines and filled symbols: exact numerical solution of the variational problem. Dashed lines and empty symbols: approximate analytical solution $\chi = \Lambda/8$. From top to bottom: lines and triangles ($\Lambda = 2.0$); lines and circles ($\Lambda = 5.0$); lines and squares ($\Lambda = 10.0$); lines and diamonds ($\lambda = 20.0$). All quantities plotted are dimensionless.
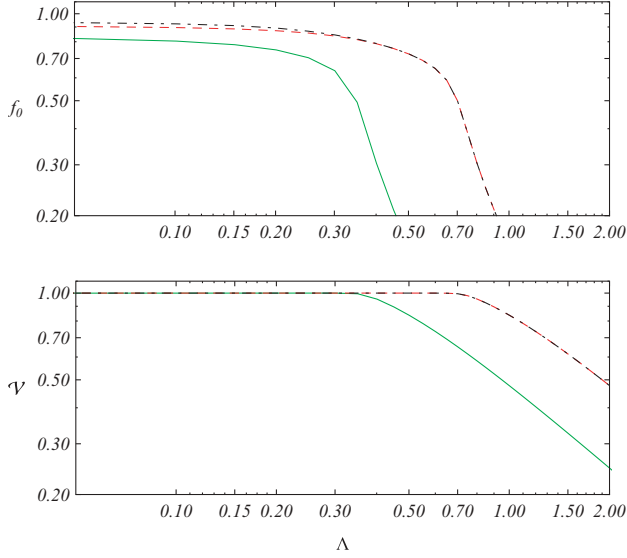
FIG. 4. (Color online) Relative atomic population ratio $f_0 = 1 - \langle n_0 \rangle / N$ (upper panel) and visibility $\mathcal{V}$ (lower panel) as functions of Λ for open chains of different size at unit filling. Solid lines: chain of $M = 11$ sites and $N = 11$ atoms. Dashed lines: chain of $M = 21$ sites and $N = 21$ atoms. Dot-dashed lines: chain of $M = 31$ sites and $N = 31$ atoms. All quantities plotted are dimensionless.

The rationale for the study of f_0 lies in the fact that it is directly associated with the visibility $\mathcal{V}$, a quantity that can be actually measured by looking at the relative difference between the maximum and the minimum of the momentum interference pattern [6]. The visibility is related to the overall coherence [20] according to the relation

$$\mathcal{V} = \frac{S_{\max} - S_{\min}}{S_{\max} - S_{\min}}, \tag{5}$$

where $S_{\max}$ and $S_{\min}$ are the maximum and minimum values of the momentum distribution function:

$$S(K) = \frac{1}{M} \sum_{l,m=1}^{M} e^{iK(l-m)} \langle a_l^\dagger a_m \rangle. \tag{6}$$

In the lower panel of Fig. 4 we report the behavior of the visibility as a function of Λ. We see that the visibility is very sensitive to the onset of localization. It is approximately constant around its maximum when the atoms are delocalized over the lattice at small values of Λ and begins to decrease exponentially, at the onset of the transition in the center of the lattice, for $\Lambda_c \simeq 0.7$.

IV. ROLE OF HIGHER BANDS

A most serious issue concerns the possibility that in the process of driving the system in the maximally excited state of the lowest energy band, the lowest states of the higher energy bands may get significantly populated. The problem is then to establish under what conditions the relative overlap between these states and the maximally excited level of the lowest band is negligible. We thus need to consider the two-band Bose-Hubbard Hamiltonian with intraband and interband interaction

terms [21]. One needs to add to the lowest-band Bose-Hubbard Hamiltonian (1) both the Bose-Hubbard Hamiltonian of the first upper energy band,

$$H_2 = \frac{U_2}{2} \sum_{j=-d}^{d} \hat{n}_j^{(2)} [\hat{n}_j^{(2)} - 1] - T_2 \sum_{j=-d}^{d-1} [\hat{a}_j^{(2)\dagger} \hat{a}_{j+1}^{(2)} + \text{H.c.}], \tag{7}$$

and the interband interaction terms

$$H_I = E_g \sum_{j=-d}^{d} \hat{n}_j^{(2)} + W \sum_{j=-d}^{d} 4\hat{n}_j \hat{n}_j^{(2)} + [\hat{a}_j^\dagger \hat{a}_j^\dagger \hat{a}_j^{(2)} \hat{a}_j^{(2)} + \text{H.c.}]. \tag{8}$$

In Eqs. (7) and (8) E_g is the energy gap between the first excited level of the optical lattice potential and the relative ground state, while $\hat{a}_j^{(2)}$, $\hat{a}_j^{(2)\dagger}$, and $\hat{n}_j^{(2)}$ are, respectively, the on-site bosonic annihilation, creation, and number operators relative to the first upper energy band. The Hamiltonian parameters of the two bands are obviously not independent: Resorting to the standard harmonic approximation for the optical lattice potential one has that $T_2 \simeq 9.4T$, $U_2 \simeq 3U/4$, and $W \simeq U/2$. Hence, the total Hamiltonian $H_T = H + H_2 + H_I$ depends only on the two independent parameters $\varepsilon = E_g/8T$, which measures the width of the energy gap, and the previously introduced $\Lambda = U(N-1)/(8T)$, which expresses the ratio of the interaction to kinetic energy scales. Going again through the same dynamical variational procedure for the two-band model H_T and finite values of the gap ε, we solve the maximization problem in the previously determined range of values of Λ that are compatible with exponential localization in the maximally excited state of the lowest energy band. As we can see from Fig. 5, the relative atomic population outside the central site f_0 is quite unaffected by the interband energy gap width until the latter becomes small enough to allow a relative population $r = \sum_{j=-d}^{d} \langle n_j' \rangle / N$ of the first upper band that is comparable with f_0. If the energy gap is further reduced, the occupation outside the central site begins to increase exponentially even if the population of the central site remains a substantial fraction of the total number of atoms until $\varepsilon \simeq \Lambda$ and $E_g \simeq U(N-1)$. This finding allows us to
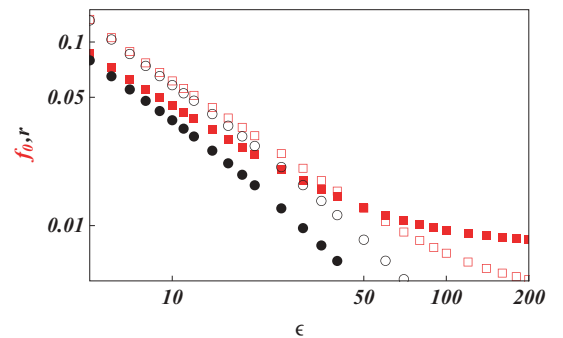

FIG. 5. (Color online) Relative atomic population outside the central site f_0 (squares) and relative population of the upper energy band r (circles) as a function of the gap width ε for different values of the energy ratio Λ. Filled symbols: $\Lambda = 2$. Empty symbols: $\Lambda = 3$. All quantities plotted are dimensionless.

conclude that if the lattice is loaded with a total number of atoms $N \leqslant E_g/(10U)$, one can safely disregard the presence of the upper energy bands.

V. CONCLUSIONS AND OUTLOOK

In conclusion, we have introduced and discussed a mechanism of exponential localization in the maximally excited state for systems of ultracold bosonic atoms with repulsive interactions in open optical lattices. The properties of the maximally excited state have been studied as a function of the Hamiltonian parameter both with numerical and analytical techniques in order to determine the region of the parameter space in which exponential localization take place and the dependence of the exponential decay on the Hamiltonian parameters. Finally, we have discussed how the transition to localization can be detected experimentally by visibility measurements, and we have established the physical conditions under which the overlap with the upper energy bands can be neglected. This localization mechanism depends on the properties of the maximally excited state that stem from the interplay of nonlinearity and a bounded energy spectrum. Because it is not a ground-state property, it does not require

the presence of random disorder, attractive local potentials, or *ad hoc* truncations of the Hilbert space.

At first sight it would seem that to populate the maximally excited state of a system in realistic experiments is an extremely challenging goal to achieve. However, thanks to the exceptional properties of controllability and manipulability of optical lattice systems, the predicted phenomenon might be observed first by cooling the system in the presence of a strong local field favoring a substantial atomic population at the center of the lattice. After switching off instantaneously the local field the system would remain, with probability close to unity, in the strongly localized maximally excited state. Repeated transitions to delocalization and exponential relocalization could then be observed simply by varying the energy ratio Λ by changing the depth of the lattice and/or by tuning the scattering length.

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