Bose-Hubbard model in a ring-shaped optical lattice with high filling factors

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The high-barrier quantum tunneling regime of a Bose-Einstein condensate confined in a ring-shaped optical lattice is investigated. By means of a change of basis transformation, connecting the set of "vortex" Bloch states and a Wannier-like set of localized wave functions, we derive a generalized Bose-Hubbard Hamiltonian. In addition to the usual hopping rate terms, such a Hamiltonian takes into account interaction-driven tunneling processes, which are shown to play a principal role at high filling factors, when the standard hopping rate parameter turns out to be negative. By calculating the energy and atomic current of a Bloch state, we show that such a hopping rate must be replaced by an effective hopping rate parameter containing the additional contribution an interaction-driven hopping rate. Such a contribution turns out to be crucial at high filling factors, since it preserves the positivity of the effective hopping rate parameter. Level crossings between the energies per particle of a Wannier-like state and the superfluid ground state are interpreted as a signature of the transition to configurations with macroscopically occupied states at each lattice site.

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I. INTRODUCTION

The study in the last decade of ultracold bosonic atoms in optical lattices has enabled the realization of an active and fruitful convergence of atomic and condensed matter physics. Particularly, the analogy of such systems with a solid material, where the bosons play the role of the superconducting electron pairs and the laser beams act as the ionic crystal, became the leitmotiv of numerous applications [1,2]. In their seminal experiment, Greiner *et al.* [3] showed that by increasing the lattice potential depth in a three-dimensional (3D) optical lattice, a quantum phase transition from a superfluid state to a Mott insulating state can be achieved. This had been predicted by Jaksch *et al.* [4], who accurately described such a transition within a Bose-Hubbard model at filling factors of the order of unity. Actually, most research has so far been focused on optical lattices with such a low filling factor, whereas the high filling factor domain appears scarcely treated. Such high filling configurations are expected to be noticeably affected by the on-site interaction between bosons, as the Wannier single-particle ground-state wave function in every site should be replaced by a macroscopic wave function [5]. A suitable configuration to experimentally investigate this type of condensate could be given by a ring-shaped lattice, where a toroidal trap becomes symmetrically divided by a number of potential barriers radiating away from the trap center [6]. In fact, apart from presenting the ideal geometry to sustain persistent currents, such a lattice would also exhibit a perfect azimuthal periodicity for any number of lattice sites. This would permit one to achieve extremely high filling factors within the present experimental possibilities for the maximum number of particles in the whole condensate. The effect of raising a single barrier across a long-lived persistent current in a toroidal condensate, has recently been investigated as the first realization of an elementary closed-loop atom circuit [7]. The generalization of such experiments to ring lattices has shown to be quite attainable in light of the works of Amico *et al.* [8] and Henderson *et al.* [9]. In fact, while the former have thoroughly discussed the experimental setup for realizing a ring lattice, such a system was actually generated by the latter, utilizing a rapidly moving laser beam that "paints" a time-averaged optical dipole potential, transforming a toroidal condensate into a ring lattice.

From a theoretical viewpoint, recent investigations have analyzed the effect of rotation on the ground-state properties of bosonic atoms confined in a one-dimensional ring lattice at low filling factors [10]. A nonrotating ring lattice, on the other hand, has been predicted to sustain persistent currents [11] if the phase difference between adjacent sites takes certain values [6]. In addition, the buildup of a winding number in the phase transition from Mott insulator to superfluid driven by a tunneling rate increase, has been shown to proceed through the so-called Kibble-Zurek mechanism, except for very slow quench times [12]. In the present work we will concentrate our attention on such nonrotating configurations with high barriers and high filling factors. The starting point of a theoretical approach to this kind of system should consist of exploring an adequate variant of the Bose-Hubbard (BH) model, which should be expected to exhibit occupation-dependent parameters [13,14]. As usual, the main ingredient to derive such a BH Hamiltonian consists in finding a suitable set of orthogonal Wannier-like functions, for which a number of variational schemes have been proposed [14–18]. Here, rather than resorting to such methods, we shall obtain our set of Wannier-like functions simply as a "basis change" from the orthogonal set of stationary "vortex" Bloch states [19,20]. Then, it will be shown that such functions possess the main properties of the single-particle Wannier functions, except for their dependence on the filling factor, and thus they become the adequate tool to study the slightly perturbed Bloch states arising from small occupation number imbalances, or from small changes in the relative phase between adjacent sites. Under such conditions, a generalized BH Hamiltonian that takes into account interaction-driven tunneling processes will be derived. Such contributions, which were previously investigated for double- and triple-well configurations [21–23], will be shown to play a principal role at high filling factors. Finally, by considering the level crossing between the energies per particle of a Wannier-like state and the superfluid ground

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state, we will discuss the transition to configurations with a macroscopic occupation at each site.

This paper is organized as follows. In Sec. II, we describe the ring lattice and remaining condensate parameters. In Sec. III, we analyze the main properties of Bloch and Wannier-like states. In Sec. IV, we derive the generalized BH Hamiltonian from which the energies of the Bloch states are calculated, and the continuity equation at a given lattice site and the corresponding atomic current are extracted. Finally, in Sec. V we discuss our numerical results for the tunneling parameters and level crossings, while in Sec. VI we present our summary and main conclusions.

II. RING-SHAPED LATTICE AND CONDENSATE PARAMETERS

We consider a Bose-Einstein condensate of rubidium atoms confined by an external trap $V_{\rm trap}$, consisting of a superposition of a toroidal term $V_{\rm toro}$ and a lattice potential $V_{\rm L}$ formed by radial barriers. Similarly to the trap utilized in recent experiments [24,25], the toroidal trapping potential in cylindrical coordinates reads

$$V_{\rm toro}(r,z) = \frac{M}{2}\left[\omega_r^2 r^2 + \omega_z^2 z^2\right] + V_0 \exp(-2\,r^2/\,\lambda_0^2), \qquad (1)$$

where ω_r and ω_z denote the radial and axial frequencies, respectively, and M denotes the atom mass. We have set $\omega_z >> \omega_r$ to suppress excitation in the z direction. In particular, we have chosen $\omega_r/(2\pi) = 7.8$ Hz and $\omega_z/(2\pi) = 173$ Hz, while for the laser beam we have set $V_0 = 100\hbar\omega_r$ and $\lambda_0 = 6\,l_r$, with $l_r = \sqrt{\hbar/(M\omega_r)}$. On the other hand, the lattice potential is formed by N_c Gaussian barriers of width λ_b and amplitude V_b, located at equally spaced angular positions $\theta_k = 2\pi k/N_c$, where $-[[(N_c-1)/2]] \leqslant k \leqslant [[N_c/2]]$ with $[[\cdot]]$ denoting the integer part,

$$V_{\rm L}(x,y) = V_b \sum_{k=-[[(N_c-1)/2]]}^{[[N_c/2]]} \Theta[\sin(\theta_k)\,y + \cos(\theta_k)\,x] \times \exp\left\{-\frac{[\cos(\theta_k)\,y - \sin(\theta_k)\,x]^2}{\lambda_b^2}\right\}, \qquad (2)$$

where Θ denotes the Heaviside function.

In the mean-field approximation, the stationary states are solutions of the Gross-Pitaevskii (GP) equation [26]:

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + V_{\rm trap}(\mathbf{r}) + g\,N|\psi(\mathbf{r})|^2\right]\psi(\mathbf{r}) = \mu\,\psi(\mathbf{r}), \qquad (3)$$

where N, μ, and $\psi(\mathbf{r})$, respectively, denote the number of particles, the chemical potential, and a two-dimensional (2D) order parameter normalized to one [27]. The effective 2D coupling constant $g = g_{3D}\sqrt{M\omega_z/2\pi\hbar}$ is written in terms of the 3D coupling constant between the atoms $g_{3D} = 4\pi a\hbar^2/M$, where $a = 98.98\,a_0$ denotes the s-wave scattering length of ^{87}Rb, a_0 being the Bohr radius.

III. BLOCH AND WANNIER-LIKE STATES

We shall restrict our treatment to the case of high enough barrier heights, where quantum tunneling between sites turns out to be the dominant dynamical process. Such a regime arises when the ground-state chemical potential becomes smaller than the minimum of the effective potential barrier dividing two lattice sites [6]. The most general solution of the GP equation (3) is given by a Bloch state of the form [19,20],

$$\psi_m(r,\theta) = e^{im\theta}\, f_m(r,\theta)\,, \qquad (4)$$

where $f_m(r,\theta)$ is invariant under rotations in $2\pi/N_c$ and the winding number m plays the role of an "angular" pseudomomentum satisfying the constraint $-[[(N_c-1)/2]] \leqslant m \leqslant [[N_c/2]]$. Such a constraint arises from the fact that all possible solutions can be reduced to those existing in the first Brillouin zone in pseudomomentum space [20]. We shall restrict ourselves to Bloch states of the lowest energy (i.e., to the ground "vortex" states [6]). In the language of crystal lattices, we would say that we shall restrict our treatment to the subspace of Bloch states of the "ground band." In such a context, the orthogonality of a pair of Bloch states, ψ_m and ψ_n, can be easily proven as follows. First, the corresponding integral may be split into separate integrals over each site, where we make the change of variable $\theta' = \theta - \theta_k$. Then, taking into account the rotational symmetry of the corresponding functions f_m and f_n, along with the equality,

$$\sum_k \exp[i(m-n)\theta_k] = \delta_{m,n} N_c\,, \qquad (5)$$

the orthogonality can be demonstrated.

Now, taking into account the periodicity of a Bloch state in the reciprocal lattice, $\psi_{m+jN_c} = \psi_m$, it must have a Fourier series expansion with "wave vectors" $\theta_k' = (\theta_k + \theta_{k+1})/2 = \theta_k + \pi/N_c$ in the direct lattice as follows [28][1]:

$$\psi_m(r,\theta) = \frac{1}{\sqrt{N_c}}\sum_k w_k(r,\theta)\, e^{i\theta_k m}\,, \qquad (6)$$

where the Fourier coefficients in (6) are given by the inversion formula[2],

$$w_k(r,\theta) = \frac{1}{\sqrt{N_c}}\sum_n \psi_n(r,\theta)\, e^{-in\theta_k}\,, \qquad (7)$$

with the summation over the angular pseudomomentum n being restricted to the first Brillouin zone. Replacing (4) in (7) and taking into account the symmetry of f_n, we may realize that the Fourier coefficients arise from a single function $w(r,\theta)$ as follows,

$$w_k(r,\theta) = w(r,\theta-\theta_k) = \frac{1}{\sqrt{N_c}}\sum_n f_n(r,\theta-\theta_k)\, e^{in(\theta-\theta_k)}\,. \qquad (8)$$

Thus, pushing forward with the analogy to crystal lattices, we could name the function,

$$w(r,\theta) = w_0(r,\theta) = \frac{1}{\sqrt{N_c}}\sum_n \psi_n(r,\theta), \qquad (9)$$

[1] Note in Eq. (6) that the phase factor $\exp(-im\pi/N_c)$ has been absorbed into the expression of the Bloch wave function.

[2] The inversion formula (7) can be readily checked by taking into account Eq. (5).

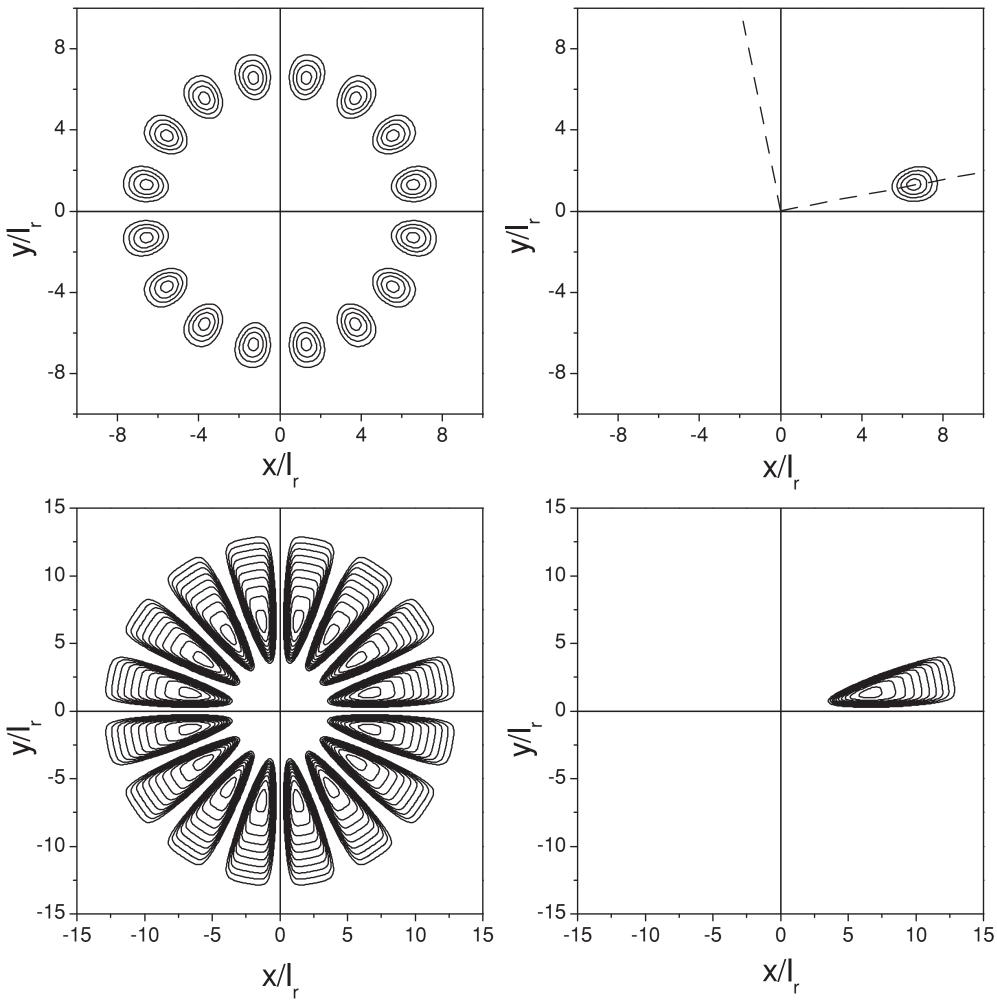

FIG. 1. Isocontours of the ground-state wave function density $|\psi_0|^2$ (left panels) and of the Wannier-like function density w^2 (right panels). The rotation of the coordinate system denoted by dashed lines in the top right panel makes the Wannier-like function symmetric with respect to the angular variable θ. The condensate parameters are $V_b/\hbar\omega_r = 10$, $N = 10^3$ (top), and $V_b/\hbar\omega_r = 80$, $N = 10^5$ (bottom), while the number of lattice sites and the Gaussian barrier width are given by $N_c = 16$ and $\lambda_b/l_r = 0.5$, respectively.

the "Wannier" function of the ground band [28]. Although we shall see that it shares many formal properties with the well-known Wannier functions, we shall also show that it presents a remarkable difference. So, we feel it is more appropriate to speak in the following of a *Wannier-like* function. Let us first show the similarities. Taking into account that the Bloch "vortex" states [20] fulfill $\psi_n^* = \psi_{-n}$, while the ground and highest states, ψ_0 and $\psi_{N_c/2}$ (N_c even), respectively, are real, it is easy to show that $w(r,\theta)$ given by (9) must be a real function. Also, from the orthonormality of the Bloch wave functions and Eq. (5), one may readily check that the set of Wannier-like functions centered on different k sites, $w(r,\theta - \theta_k)$, form indeed an orthonormal basis of the subspace of Bloch states of the ground band. In addition, given that the Bloch "vortex" states fulfill $\psi_n(r,-\theta) = \psi_n^*(r,\theta)$, it is easy to show that $w(r,\theta)$ turns out to be an even function of θ for odd N_c. On the other hand, by considering the rotation of the coordinate system in π/N_c shown in Fig. 1, which makes the Bloch wave function $\psi_{N_c/2}(r,\theta)$ an even function of θ, the same parity property may be readily extended to the case of N_c even. Finally, by replacing the numerical solutions of the GP equation, $\psi_n(r,\theta)$, in Eq. (9), we have shown that our Wannier-like function is indeed a well-localized one, as seen in Fig. 1. However, there is a most remarkable difference between such a localized function and a "true" Wannier function, which consists in that only the former turns out to depend on the filling factor (i.e., the average number of particles at each site), as clearly observed in Fig. 1. In fact, only for noninteracting bosons our Wannier-like function would not depend on the filling factor. We have performed a calculation of the overlap between the Wannier-like function given by (9) and the corresponding Wannier-like function for noninteracting bosons (i.e., with a vanishing coupling constant $g = 0$), which yielded 1.00, 0.98, and 0.48, for filling factors 5, 62.5, and 6250, respectively. Particularly, the last two values correspond to the filling factors of the top and bottom panels of Fig. 1, respectively. Therefore, we may conclude that only for filling factors below $\sim$60, the Wannier-like functions should be almost independent of the average occupation number. We will have more to say about this filling factor dependence in the following sections.

To conclude it is instructive to rewrite Eq. (6) as

$$\psi_m(r,\theta) = \frac{1}{\sqrt{N_c}} \sum_k w(r,\theta-\theta_k)\, e^{im\theta_k}\,, \tag{10}$$

and notice that the above representation will be accurate to the extent that each site presents an almost uniform phase, which is consistent with a tight-binding scenario of high barriers with a low particle current [6].

IV. BOSE-HUBBARD MODEL

The above similarities between the Wannier-like function and the "true" Wannier functions, offer the adequate framework to establish a BH model for our ring-shaped optical lattice. As usual [2,4,29], the starting point is the second-quantized Hamiltonian,

$$\begin{aligned}\hat{H} &= \int d^2\mathbf{r}\ \hat{\Psi}^\dagger(\mathbf{r})\left[-\frac{\hbar^2}{2M}\nabla^2 + V_{\rm trap}(\mathbf{r})\right]\hat{\Psi}(\mathbf{r})\\ &\quad + \frac{g}{2}\int d^2\mathbf{r}\ \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Psi}(\mathbf{r}),\end{aligned} \tag{11}$$

where $\hat{\Psi}(\mathbf{r})$ is the boson field operator. We are interested in slightly perturbed Bloch states, which could be given by, for example, a small relative imbalance between the average population of two neighboring sites. Then, for low enough temperatures, such configurations will be conveniently described by expanding the field operators in our Wannier-like basis of the ground band,

$$\hat{\Psi}(\mathbf{r}) = \sum_k w(r,\theta-\theta_k)\,\hat{a}_k, \tag{12}$$

where the operator $\hat{a}_k$ destroys a particle in the k-Wannier state and satisfies the usual Bose commutation relations. Here we remark that a possible dependence of the operators $\hat{a}_k$ on the filling factor should, under the above conditions, be negligible. In fact, in the previous section we have seen that this is actually the case for filling factors below ∼60, while for higher fillings, only configurations that present small population imbalances should be taken into consideration.

Then, replacing the field operators in (11) through Eq. (12) and assuming the tight-binding limit, where only the coupling to the nearest neighboring states of any given Wannier-like state is taken into account, we obtain the following BH Hamiltonian:

$$\begin{aligned}\hat{H}_{\rm BH} &= \varepsilon\sum_k \hat{a}_k^\dagger\hat{a}_k - J\sum_k(\hat{a}_k^\dagger\hat{a}_{k+1} + \hat{a}_{k+1}^\dagger\hat{a}_k)\\ &\quad - \frac{J'}{2}\sum_k[\hat{a}_k^\dagger\hat{a}_k^\dagger\hat{a}_k(\hat{a}_{k+1}+\hat{a}_{k-1})\\ &\quad + (\hat{a}_{k+1}^\dagger + \hat{a}_{k-1}^\dagger)\hat{a}_k^\dagger\hat{a}_k\hat{a}_k] + \frac{U}{2}\sum_k \hat{a}_k^\dagger\hat{a}_k^\dagger\hat{a}_k\hat{a}_k,\end{aligned} \tag{13}$$

with

$$\varepsilon = \int d^2\mathbf{r}\ w(r,\theta)\left[-\frac{\hbar^2}{2M}\nabla^2 + V_{\rm trap}(\mathbf{r})\right]w(r,\theta), \tag{14}$$

$$J = -\int d^2\mathbf{r}\ w(r,\theta)\left[-\frac{\hbar^2}{2M}\nabla^2 + V_{\rm trap}(\mathbf{r})\right]w(r,\theta\pm 2\pi/N_c), \tag{15}$$

$$J' = -2\,g\int d^2\mathbf{r}\ w^3(r,\theta)\,w(r,\theta\pm 2\pi/N_c), \tag{16}$$

$$U = g\int d^2\mathbf{r}\ w^4(r,\theta), \tag{17}$$

where the equivalence between the "±" expressions at the right-hand side of (15) stems from the reality of the Wannier-like functions, while the corresponding equivalence in (16) results from the parity property of such functions. In addition to the usual tunneling terms proportional to the standard hopping rate J, we have also retained in (13) interaction terms up to the first order in the product of adjacent Wannier-like functions, which are proportional to the tunneling parameter J'[3]. Later we will show that such interaction terms may constitute the most significant contribution to the tunneling rate at high filling factors. The case of two sites $N_c = 2$ is somewhat special since it is the only configuration presenting a single neighbor for each site. Then, the expression (13) reduces to

$$\begin{aligned}\hat{H}_{\rm BH} &= \varepsilon\hat{N} - \left[J + \frac{(\hat{N}-1)}{N_c}J'\right](\hat{a}_0^\dagger\hat{a}_1 + \hat{a}_1^\dagger\hat{a}_0)\\ &\quad + \frac{U}{2}(\hat{a}_0^\dagger\hat{a}_0^\dagger\hat{a}_0\hat{a}_0 + \hat{a}_1^\dagger\hat{a}_1^\dagger\hat{a}_1\hat{a}_1),\end{aligned} \tag{18}$$

where, for a fixed number of bosons N, the particle number operator $\hat{N} = \hat{a}_0^\dagger\hat{a}_0 + \hat{a}_1^\dagger\hat{a}_1$ may be replaced by a c number. Thus, we may see that the only difference with the standard two-mode BH Hamiltonian consists in that the standard hopping rate J is replaced by an effective hopping rate,

$$J_{\rm eff} = J + \frac{(N-1)}{N_c}J', \tag{19}$$

which includes the additional contribution of an interaction-driven hopping rate $\frac{N-1}{N_c}J'$ stemming from boson interactions. Here it is worth noticing that an extended two-mode approach, which includes terms in the BH Hamiltonian beyond the present approximation, has been recently investigated [21,30].

Next we obtain the mean value of the BH Hamiltonian $\langle N,m|\hat{H}_{BH}|N,m\rangle$, where $|N,m\rangle$ represents the quantum state of N bosons condensed in the Bloch state (4) of the winding number m [19,20]. To calculate such a matrix element, we may change to the Bloch basis in (13) by means of the expansion [cf. (7)],

$$\hat{a}_k^\dagger = \frac{1}{\sqrt{N_c}}\sum_n \hat{\alpha}_n^\dagger\, e^{-in\theta_k}\,, \tag{20}$$

where the operator $\hat{\alpha}_n^\dagger$ creates a particle in the corresponding Bloch state. Then, a straightforward calculation yields

$$\begin{aligned}E_m &\equiv \langle N,m|\hat{H}_{\rm BH}|N,m\rangle/N = \varepsilon + \frac{(N-1)}{N_c}\frac{U}{2}\\ &\quad - \nu J_{\rm eff}\cos(2\pi m/N_c),\end{aligned} \tag{21}$$

where ν denotes the number of neighbors ($\nu = 2$ ($\nu = 1$) for $N_c > 2$ ($N_c = 2$)). We note that the above expression coincides with our previous result [6] in the limit $N \gg 1$.

[3]We have ignored in (13) nearest-neighbor repulsion terms [33] because they are of second order in the product of adjacent Wannier-like functions.

It is instructive to analyze the continuity equation for the kth site of a lattice with $N_c > 2$,

$$\frac{d}{dt}(\hat{a}_k^\dagger \hat{a}_k) = \frac{i}{\hbar}[\hat{H}_{\rm BH},\hat{a}_k^\dagger \hat{a}_k] = \hat{J}_{k-1\to k} - \hat{J}_{k\to k+1}, \tag{22}$$

where $\hat{J}_{k\to k+1}$ denotes the current operator for atoms that move from site k to site $k+1$,

$$\hat{J}_{k\to k+1} = \frac{i}{\hbar}\left(\hat{a}_{k+1}^\dagger \hat{J}_{\rm eff}^{(k)} \hat{a}_k - \hat{a}_k^\dagger \hat{J}_{\rm eff}^{(k)} \hat{a}_{k+1}\right), \tag{23}$$

which has been written in terms of the hopping operator between sites k and $k+1$ defined by

$$\hat{J}_{\rm eff}^{(k)} = J + \frac{J'}{2}(\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{k+1}^\dagger \hat{a}_{k+1}). \tag{24}$$

The mean value of the current operator (23) for a condensate of N particles in the Bloch state of the winding number m reads

$$\langle N,m|\hat{J}_{k\to k+1}|N,m\rangle = 2J_{\rm eff}\frac{N}{N_c}\sin(2\pi m/N_c), \tag{25}$$

which does not depend on the site we are considering, as expected. Note that analogously to the mean value of the angular momentum [6], the current turns out to be a sinusoidal function of the winding number. Note also its proportionality to the effective hopping rate $J_{\rm eff}$, whereas for the standard BH model such a current turns out to be proportional to the standard hopping rate J [31].

The value of the BH model parameters (14)–(17) can be easily extracted from the mean-field energy of Bloch states $\mathcal{E}_m$ (see Appendix A). Particularly, from the single value of energies of the ground state $\mathcal{E}_0$ and the highest excited state $\mathcal{E}_{N_c/2}$ (N_c even) one obtains

$$\varepsilon = \frac{1}{2}\left(\mathcal{E}_{N_c/2}^0 + \mathcal{E}_0^0\right), \tag{26}$$

$$U = \frac{N_c}{N-1}\left(\mathcal{E}_{N_c/2}^{\rm int} + \mathcal{E}_0^{\rm int}\right), \tag{27}$$

$$J = \frac{1}{2\nu}\left(\mathcal{E}_{N_c/2}^0 - \mathcal{E}_0^0\right), \tag{28}$$

$$J' = \frac{N_c}{2\nu(N-1)}\left(\mathcal{E}_{N_c/2}^{\rm int} - \mathcal{E}_0^{\rm int}\right), \tag{29}$$

where, according to Appendix A, the superscripts "int" and "0" denote interacting and noninteracting contributions to the energy, respectively.

According to the Hamiltonian (13), the energy per particle in a Wannier-like state (i.e., neglecting tunneling processes) is given by

$$E_W = \varepsilon + \frac{U}{2}\left(\frac{N}{N_c} - 1\right). \tag{30}$$

It is interesting to compare the above energy to the energy per particle of the superfluid ground state E_0. Then, from Eqs. (21) and (30) we obtain

$$E_W - E_0 = \nu J_{\rm eff} - \left(\frac{N_c - 1}{N_c}\right)\frac{U}{2}. \tag{31}$$

The existence of a superfluid to Mott-insulator transition requires the above difference to be positive for low barrier heights (superfluid regime), and negative for high barrier heights (Mott-insulator state). Thus, the level crossing at an intermediate barrier height arising from (31), should be representing a transition to configurations where the system is well described by N_c macroscopically occupied states. We may utilize the above expression to obtain the value at such a level crossing, $\eta_{\rm cr}$, of the dimensionless scaling parameter [2,29]

$$\eta = \frac{U}{\nu J_{\rm eff}}, \tag{32}$$

relevant to the superfluid to Mott-insulator transition. Thus, assuming $E_W = E_0$ in (31), we obtain

$$\eta_{\rm cr} = 2N_c/(N_c - 1). \tag{33}$$

We may compare the above result with theoretical estimates focusing on critical values of the parameter U/J. In fact, it has been pointed out that the superfluid to Mott-insulator transition in a one-dimensional BH model can be described by the (1 + 1)D O(2) model, which gives [1]

$$(U/J)_{\rm cr} = 2.2\,\bar{n} \tag{34}$$

for filling factors $\bar{n} \gg 1$. The above proportionality to the filling factor is also predicted from the mean-field Gutzwiller ansatz, which yields $(U/J)_{\rm cr} = 2(\sqrt{\bar{n}} + \sqrt{\bar{n}+1})^2 \simeq 8\,\bar{n}$ for $\bar{n} \gg 1$ [10]. However, we must recall that mean-field theories only provide a qualitative analysis in 1D systems. We must also remark that the result (34) arises from a BH Hamiltonian that does not take into account the contribution of the interaction-driven tunneling terms proportional to J'. So, such an estimate should only be reliable for $J_{\rm eff} \simeq J$ [i.e., for $J \gg \bar{n}J'$ ($\bar{n} \gg 1$)]. However, we shall see in the following section that such conditions are difficult to reach within our condensate parameters. Moreover, we shall show that the standard hopping rate J becomes negative above a certain filling factor, which means that the parameter U/J should actually increase with the average occupation number until becoming divergent and meaningless above such a filling factor.

V. NUMERICAL RESULTS

In the BH model for linear lattices it is common to measure energies in units of the *recoil energy* $E_R = \hbar^2 k_B^2/2M$, where the Bragg momentum k_B corresponds to a lattice potential of the form $\sim\sin^2(k_B\,x)$. To adapt this definition to the present case, we first note that a lattice potential $\sim\sin^2(N_c\,\theta/2)$ would have the required angular periodicity of $2\pi/N_c$. Then, recalling that without barriers the excitation energy per particle of a Bloch state of angular pseudomomentum m reads Km^2, where [6]

$$K = \frac{\pi\hbar^2}{M}\int \frac{1}{r}[\psi_0(r)]^2 dr, \tag{35}$$

we may realize that our "recoil energy" should be written

$$E_R = K(N_c/2)^2. \tag{36}$$

We have performed numerical simulations for three particle numbers, $N = 80$, 10^3, and 10^5; given that the corresponding recoil energies turned out to be $0.743\ \hbar\omega_r$, $0.740\ \hbar\omega_r$, and $0.713\ \hbar\omega_r$, respectively, showing figures that approximate the harmonic energy quantum $\hbar\omega_r$, we decided, for the sake of simplicity, to keep such a value as our energy unit in all cases.

TABLE I. Level crossings arising from Eq. (31); see text for explanation.

N_c	N	N/N_c	$V_b/\hbar\omega_r$	$V_{\min}/\mu_0$	μ/μ_0	$\eta_{\rm cr}$	$V_b/\hbar\omega_r$ [1]
16	80	5	10.4	1.29	1.05	2.17	14.1
	10^3	62.5	15.4	1.39	1.08	2.18	30
	10^5	6250	95.4	1.72	1.25	2.23	
8	80	10	4.65	1.11	1.01	2.29	8.2
	10^3	125	10.1	1.23	1.03	2.30	15.2
	10^5	12500	81.4	1.53	1.11	2.32	
4	80	20	2.95	1.06	1.00	2.23	5.8
	10^3	250	8.93	1.20	1.01	2.68	
	10^5	25000	77.1	1.47	1.05	2.48	

We have numerically evaluated the BH parameters through Eqs. (26)–(29) for the above particle numbers and three numbers of lattice sites, $N_c = 16$, 8, and 4. In Table I, we display our numerical estimates for the level crossings for the different condensates and a Gaussian barrier width $\lambda_b/l_r = 0.5$. Apart from the dependence of the barrier height parameter V_b, it is interesting to compare the minimum of the effective potential barrier dividing two lattice sites $V_{\min}$ [6], with the ground-state chemical potential μ. Recall that in Ref. [6] we have identified the lower bound of the quantum tunneling regime as $V_{\min}/\mu \simeq 1$. To scale out the dependence of the barrier height for different particle numbers, we have represented $V_{\min}$ and μ in units of the chemical potential at zero barrier μ_0 for each particle number. Compare also the numerical estimates for η_{cr} shown in Table I to those given by the expression (33), namely $\eta_{\rm cr} = 2.13$, 2.29, and 2.67 for $N_c = 16$, 8, and 4, respectively. Here it is worthwhile pointing out that a similar agreement was found for wider Gaussian barriers ($\lambda_b/l_r = 1$). Finally, the last column of Table I shows the critical estimate for the barrier height parameter V_b arising from Eq. (34). The absence of data for filling factors above 125 corresponds to the negative values obtained for the hopping rate J. Note also that such critical barrier heights turn out to be always higher than those of the fourth column, as expected.

In Figs. 2 and 3 we depict the standard hopping rate J (15) computed from Eq. (28), the tunneling parameter $\frac{N-1}{N_c}J'$ (16) computed from Eq. (29), and their sum $J_{\rm eff}$, as functions of the barrier height. Particularly, Fig. 2 shows that while the interaction component $\frac{N-1}{N_c}J'$ turns out to be almost negligible for 80 particles and $N_c = 16$ (filling factor = 5), for fewer lattice sites it shows a relative increase until becoming of the same order of the hopping rate J for $N_c = 4$ (filling factor = 20). The larger filling factors of $N = 10^3$ yield an interaction component that turns out to be always larger than the standard hopping rate, to such an extent that J eventually becomes negative for $N_c = 4$. Note that such a dramatic change of sign occurs in between fillings of 125 and 250 particles (Table I). Negative values of J were also predicted by Ananikian *et al.* for large atom numbers in a double-well condensate [21]. Finally, the extremely high fillings of $N = 10^5$ yield again a negative J, as expected, while a sort of saturation in the relative weights of the interaction component and the negative hopping rate is observed. This is reflected through the quite similar plots of Fig. 3, despite the vertical shift for varying N_c, which arises

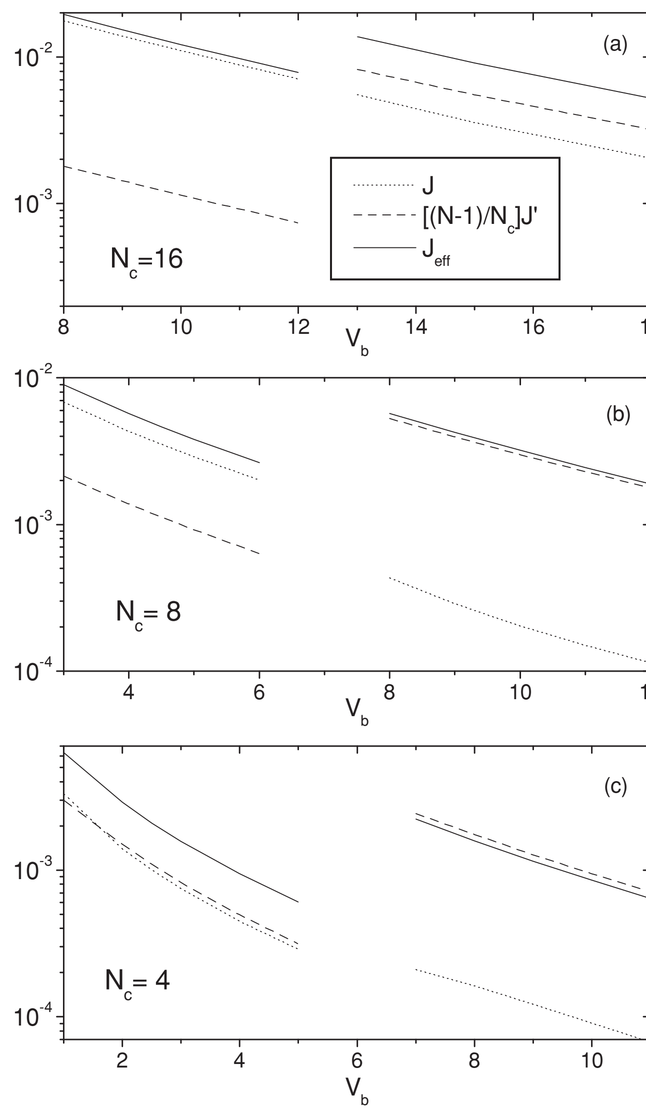

FIG. 2. Standard hopping rate J, interaction-driven hopping rate $\frac{N-1}{N_c}J'$, and effective hopping rate $J_{\rm eff}$, as functions of the barrier height V_b for the condensates of 80 particles (left) and 10^3 particles (right). All quantities are given in units of $\hbar\omega_r$. In panel (c) the standard hopping rate J turns out to be negative for 10^3 particles (right), so we have depicted its absolute value $|J|$.

from a decrease of the probability of tunneling events as the number of barriers is lowered.

To conclude this section, we display in Fig. 4 the dimensionless scaling parameter $\eta = U/(\nu J_{\rm eff})$ versus the barrier height, for each number of particles and $N_c = 16$. Notice that quite similar ranges of η are obtained irrespective of the barrier height interval, and this behavior repeats for the remaining values of N_c.

VI. SUMMARY AND CONCLUDING REMARKS

We have analyzed the high-barrier quantum tunneling regime of a Bose-Einstein condensate confined in a ring-shaped optical lattice. Representing the orthogonal set of "vortex" Bloch states through a basis of well-localized Wannier-like functions, we were able to formulate a variant of the

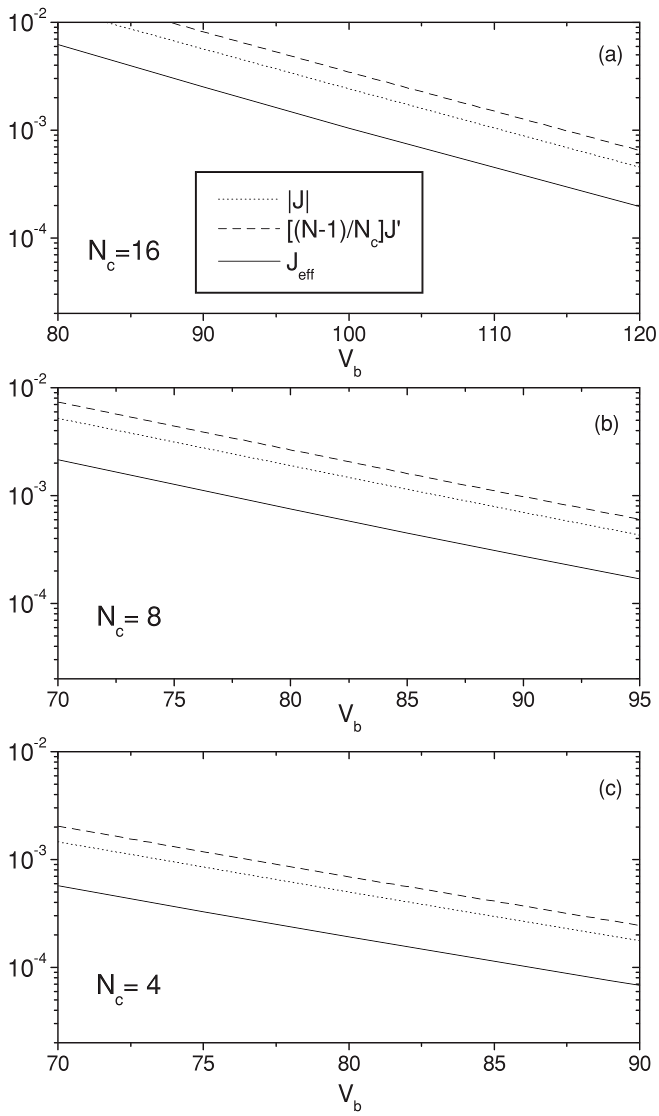

FIG. 3. Absolute value of the standard hopping rate $|J|$, interaction-driven hopping rate $\frac{N-1}{N_c}J'$, and effective hopping rate $J_{\rm eff}$, as functions of the barrier height V_b for the condensate of 10^5 particles. All quantities are given in units of $\hbar\omega_r$.

Bose-Hubbard model, adequate for slightly perturbed Bloch states at any filling factor. In addition to the usual hopping rate terms, such a Hamiltonian contains interaction-driven tunneling terms, which are shown to play its most important role when the standard hopping rate parameter becomes negative at high filling factors. In fact, by calculating the energy and atomic current of a Bloch state, we have shown that the standard hopping rate parameter must be replaced by an effective hopping rate containing the additional contribution from the interaction-driven tunneling terms in the BH Hamiltonian. We remark the importance of such an interaction-driven hopping rate parameter, since it is shown to preserve the positivity of the effective hopping rate at high filling factors. A quite similar behavior for such hopping rates was recently predicted for large atom numbers in a two-well configuration [21].

We have found that, as the barrier height is increased, the energies per particle of a Wannier-like state and the condensate ground state exhibit a level crossing, which is interpreted as a signature of the transition to configurations with macroscopically occupied states at each lattice site. It is also shown that the dimensionless scaling parameter, relevant to the superfluid to Mott-insulator transition, takes a remarkably simple expression at the level crossing, which only depends on the number of lattice sites.

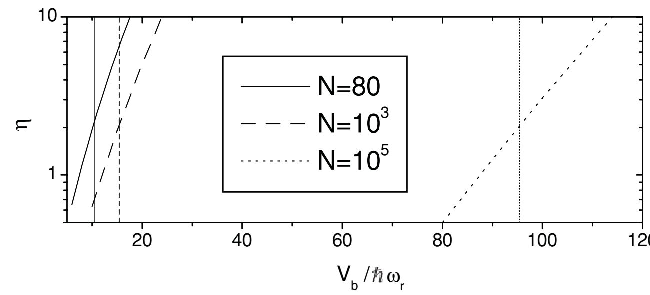

FIG. 4. Dimensionless scaling parameter $\eta = U/(\nu J_{\rm eff})$ as a function of the barrier height V_b for $N_c = 16$ and the condensates of 80, 10^3, and 10^5 particles. The vertical lines correspond to values in the fourth column of Table I.

Finally, we would like to point out that a future direction of the present studies will consist of exploring the Boson Josephson–junction dynamics described by a generalized N_c-mode GP equation [21,22,32].

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APPENDIX: ALTERNATIVE CALCULATION OF THE BH MODEL PARAMETERS

An alternative calculation of the BH model parameters (14)–(17), which avoids changing to a smaller numerical grid to deal with the tiny regions where the integrands of the tunneling parameters (15) and (16) are nonvanishing, proceeds as follows. The method rests on the calculation of the mean-field energies of the Bloch states $\mathcal{E}_m$, which are obtained by numerically solving the GP equation (3) for the order parameters ψ_m [6], in order to evaluate the integral yielding the energy per particle,

$$\mathcal{E}_m = \int \left(\frac{\hbar^2}{2M} |\nabla \psi_m|^2 + V_{\rm trap}\, |\psi_m|^2 + \frac{1}{2} N g\, |\psi_m|^4 \right) dx\, dy, \tag{A1}$$

where we may distinguish noninteracting and interacting contributions,

$$\mathcal{E}_m^0 = \int \left(\frac{\hbar^2}{2M} |\nabla \psi_m|^2 + V_{\rm trap}\, |\psi_m|^2 \right) dx\, dy, \tag{A2}$$

and

$$\mathcal{E}_m^{\rm int} = \int \frac{1}{2} N g\, |\psi_m|^4 dx\, dy, \tag{A3}$$

respectively. In the context of this paper (i.e., for large barrier heights), the above GP energies (A2)–(A3) must coincide with those given by the corresponding contributions in (21) with $J_{\rm eff}$ replaced from (19). Then, by calculating (A2)–(A3) for any two Bloch states and equating such results to the corresponding terms in (21), one can construct a linear system of four equations from which we may obtain the BH model parameters (14)–(17). For instance, the simplest choice for N_c even corresponds to the winding numbers $m = 0$ and $m = N_c/2$, which yields the following set of equations:

$$\mathcal{E}_0^0 = \varepsilon - \nu J, \tag{A4}$$

$$\mathcal{E}_0^{\rm int} = \frac{(N-1)}{N_c}(U/2 - \nu J'), \tag{A5}$$

$$\mathcal{E}_{N_c/2}^0 = \varepsilon + \nu J, \tag{A6}$$

$$\mathcal{E}_{N_c/2}^{\rm int} = \frac{(N-1)}{N_c}(U/2 + \nu J'), \tag{A7}$$

and the solution of such a system is given by the expressions (26)–(29).

Finally, a similar calculation for N_c odd yields

$$\varepsilon = \left[\mathcal{E}_{(N_c-1)/2}^0 + \mathcal{E}_0^0 \cos(\pi/N_c)\right]/[1+\cos(\pi/N_c)], \tag{A8}$$

$$U = \frac{2N_c}{N-1}\left[\mathcal{E}_{(N_c-1)/2}^{\rm int} + \mathcal{E}_0^{\rm int} \cos(\pi/N_c)\right]/[1+\cos(\pi/N_c)], \tag{A9}$$

$$J = \frac{1}{2}\left[\mathcal{E}_{(N_c-1)/2}^0 - \mathcal{E}_0^0\right]/[1+\cos(\pi/N_c)], \tag{A10}$$

$$J' = \frac{N_c}{2(N-1)}\left[\mathcal{E}_{(N_c-1)/2}^{\rm int} - \mathcal{E}_0^{\rm int}\right]/[1+\cos(\pi/N_c)]. \tag{A11}$$

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