Ultracold Lattice Gases with Periodically Modulated Interactions

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We show that a time-dependent magnetic field inducing a periodically modulated scattering length may lead to interesting novel scenarios for cold gases in optical lattices, characterized by a nonlinear hopping depending on the number difference at neighboring sites. We discuss the rich physics introduced by this hopping, including pair superfluidity, exactly defect-free Mott-insulator states for finite hopping, and pure holon and doublon superfluids. We also address experimental detection, showing that the introduced nonlinear hopping may lead in harmonically trapped gases to abrupt drops in the density profile marking the interface between different superfluid regions.

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Ultracold atoms in optical lattices formed by laser beams provide an excellent environment for studying lattice models of general relevance in condensed-matter physics, and in particular, variations of the celebrated Hubbard model [1,2]. Cold lattice gases allow for an unprecedented degree of control of various experimental parameters, even in real time. In particular, interparticle interactions can be changed by means of Feshbach resonances [3]. Moreover, recent milestone achievements allow for site-resolved detection, permitting the study of *in situ* densities [4,5], and more involved measurements, as that of nonlocal parity order [6].

The modulation of the lattice parameters in real time opens interesting possibilities of control and quantum engineering. In particular, a periodic lattice shaking translates by means of Floquet's theorem [7,8] into a modified hopping constant [9], which may even reverse its sign as shown in experiments [10,11]. This technique has been employed to drive the Mott-insulator (MI) to superfluid (SF) transition [12], and to simulate frustrated classical magnetism [13]. Recent experiments have explored as well the fascinating perspectives offered by periodically driven lattices in strongly correlated gases [14,15].

The effective Hubbard-like models describing ultracold lattice gases are typically characterized by a hopping independent of the number of particles at the sites. This is, however, not necessarily the case. Multiband physics [16–18] and dipolar interactions for sufficiently large dipole moments [19] may lead to occupation-dependent hopping. A major consequence of nonlinear hopping is the possibility to observe pair superfluidity (PSF) [19,20], which resembles pairing in SF Fermi gases, although for bosons superfluidity exists as well without pairing.

In this Letter, we consider a cold lattice gas in the presence of a periodically modulated magnetic field. In the vicinity of a Feshbach resonance, this field induces modulated interparticle interactions [21]. Interestingly, Ref. [22] has shown that periodic modulations of the interaction strength may lead to a many-body coherent destruction of tunneling in two-mode Bose-Einstein condensates. As shown below, the generalization of this effect to lattice gases leads under proper conditions to an effective Hubbard-like model with a nonlinear hopping which, in contrast to other proposals mentioned above, depends on the difference of occupations at neighboring sites, and retains its nonlinear character even for weak lattices. We discuss the rich physics introduced by this hopping, including pair superfluid phases, exactly defect-free MI states for finite hopping, and pure holon and doublon superfluids. We also address experimental detection, showing that the studied nonlinear hopping may lead to abrupt drops in the density profile of harmonically trapped gases.

We consider bosons in a lattice in the presence of a periodically modulated magnetic field $B(t) = B(t + T)$ (with period $T = 2\pi/\omega$) chosen close to a Feshbach resonance, where the s-wave scattering length acquires the form $a(t) = a_{bg}(1 - \frac{\Delta B}{B(t)-B_r}) = a_0 + \sum_{l>0} a_l \cos(l\omega t)$. Here ΔB and B_r determine the width and position of the resonance, respectively, and a_{bg} is the background scattering length [3]. Assuming that the gap between the first two lattice bands is much larger than any other energy scale in the problem, we consider only the lowest band and describe the system by a Bose-Hubbard model (BHM) [1,2]:

$$H(t) = -J\sum_{\langle ij\rangle} b_i^\dagger b_j + \frac{U(t)}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \sum_i \mu \hat{n}_i, \quad (1)$$

where b_i ($b_i^\dagger$) is the bosonic annihilation (creation) operator at site i, $\hat{n}_i = b_i^\dagger b_i$, μ is the chemical potential, $J > 0$ is the hopping rate, and $\langle..\rangle$ denotes nearest neighbors. Interactions are characterized by a coupling $U(t) = U_0 + \sum_{l>0} U_l \cos(l\omega t) = U_0 + \tilde{U}(t)$, with $U_0 > 0$ and $U_l = \frac{4\pi\hbar^2 a_l}{M}\int d^3r |w(\mathbf{r})|^4$. Here $w(\mathbf{r})$ is the lowest Wannier function and M is the atomic mass.

We apply a similar analysis as the one used for shaken lattices [9]. We specify a Floquet basis

$$|\{n_j\}, m\rangle = e^{im\omega t} e^{-(iV(t)/2)\sum_j \hat{n}_j(\hat{n}_j - 1)} |\{n_j\}\rangle, \qquad (2)$$

where m defines the Floquet sectors and $|\{n_j\}\rangle$ is the Fock basis, characterized by the atom number at each site. In Eq. (2), we defined $V(t) = \int^t \tilde{U}(t')dt'/\hbar$. We introduce the time-averaged scalar product $\langle\langle\{n_j'\}, m'|\ldots|\{n_j\}, m\rangle\rangle = \frac{1}{T}\int_0^T \langle\{n_j'\}, m'|\ldots|\{n_j\}, m\rangle$, and establish the matrix elements:

$$\begin{aligned}&\langle\langle\{n_j'\}, m'|[H(t) - i\hbar\partial_t]|\{n_j\}, m\rangle\rangle \\ &\quad = \delta_{m,m'}\langle\{n_j'\}|H_m|\{n_j\}\rangle \\ &\quad\quad - J\sum_{\langle i,j\rangle}\langle\{n_j'\}|b_i^\dagger F_{m'-m}(\hat{n}_i - \hat{n}_j)b_j|\{n_j\}\rangle, \qquad (3)\end{aligned}$$

with $H_m = m\hbar\omega + \frac{U_0}{2}\sum_j \hat{n}_j(\hat{n}_j - 1) - \sum_j \mu\hat{n}_j$ and $F_m(x) = \frac{1}{T}\int_0^T dt e^{-imt} e^{iV(t)x}$. If $\hbar\omega \gg J$, U_0, we may restrict to a single Floquet sector $m = 0$, resulting in an effective time-independent Hamiltonian of the form

$$H_{\rm eff} = -J\sum_{\langle ij\rangle} b_i^\dagger F_0(\hat{n}_i - \hat{n}_j)b_j + \frac{U_0}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu\sum_i \hat{n}_i. \qquad (4)$$

Hence, interactions with a periodic modulation result in a nonlinear hopping term, which depends on the atom number difference between neighboring sites. Note that this nonlinear character remains relevant for any value of the bare hopping J. In the following we discuss the specific case $\tilde{U}(t) = U_1\cos\omega t$. In this case, $F_0(x) = \mathcal{J}_0(\Omega x)$, with $\mathcal{J}_0$ the Bessel function and $\Omega = U_1/\hbar\omega$, generalizing the result of Ref. [22] for two-well Bose-Einstein condensates.

Insight into Eq. (4) is gained by means of a Gutzwiller ansatz (GA) for the ground state [23], $|G\rangle = \prod_j\sum_n f_n(j)|n_j\rangle$, where $f_n(j)$ are variational parameters $[\sum_n |f_n(j)|^2 = 1]$, determined by minimizing $\langle G|H_{\rm eff}|G\rangle$. Results obtained by choosing homogeneous real $f_n(j) = f_n$

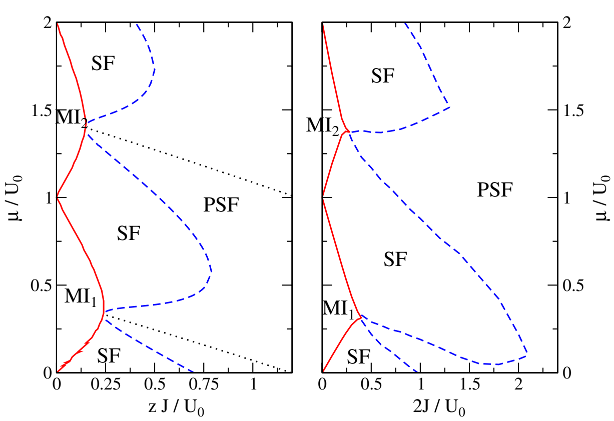

FIG. 1 (color online). Phase diagram for $\Omega = 4$ using the GA (left) and the DMRG (right). Solid curves define the MI lobes, whereas dashed curves are the SF-PSF boundaries. The black dotted line indicates $\langle b_i\rangle = 0$.

[24] are shown in Fig. 1 (left), where we depict the mean-field phase diagram for $\Omega = 4$ $[\mathcal{J}_0(\Omega) \simeq -0.4]$ as a function of μ/U_0 and zJ/U_0, with z the coordination number. As usual, MI phases are characterized by integer $\langle\hat{n}_i\rangle$, and vanishing single-particle- and pair-condensation fractions, $\rho_1 \equiv |\langle b_i\rangle|^2/\langle\hat{n}_i\rangle$ and $\rho_2 = |\langle b_i^2\rangle|^2/\langle\hat{n}_i\rangle^2$. The superfluid regime may be split into two different phases separated by a crossover: a usual bosonic superfluid, characterized by a dominant single-particle condensation, $\rho_1 > \rho_2 > 0$, and a pair superfluid, where pair-condensation dominates, $\rho_2 > \rho_1 \geq 0$. Pair superfluidity is especially pronounced in the vicinity of integer $\langle\hat{n}_i\rangle$, where $\langle b_i\rangle = 0$. Our GA results show that PSF only occurs if $\mathcal{J}_0(\Omega) < 0$. This may be understood by considering integer $\langle\hat{n}\rangle = n$, and restricting the variational space to $f_{n\pm1} = \frac{\sin\eta}{\sqrt{2}}e^{i\varphi_\pm}$ and $f_n = \cos\eta$. For $\mathcal{J}_0(\Omega) < 0$, energy minimization gives $\bar{\varphi} \equiv \varphi_+ + \varphi_- = \pi$, while $\bar{\varphi} = 0$ for $\mathcal{J}_0(\Omega) > 0$. As a result, for $2Jz/U_0 \gg 1$, PSF demands $(n+1) > 2(\sqrt{n} + \mathrm{sgn}(\mathcal{J}_0(\Omega))\sqrt{n+1})^2$, which is only fulfilled if $\mathcal{J}_0(\Omega) < 0$.

To complement the mean-field GA results, we have also employed numerically exact methods in one dimension. In particular, we used the density-matrix renormalization group (DMRG) [25] with up to 40 sites and keeping 200 states, and a related method, the infinite time-evolving block decimation (iTEBD) method [26] using a Schmidt dimension of 200. We have monitored the behavior of single-particle and pair correlations, $G_1(i,j) \equiv \langle b_i^\dagger b_j\rangle$ and $G_2(i,j) \equiv \langle(b_i^\dagger)^2 b_j^2\rangle$, respectively. Both decay exponentially in the Mott insulator. For both the PSF and SF regions, both G_1 and G_2 have a power-law decay [27], but in the PSF G_2 decays slower than G_1. The opposite characterizes the SF phase. Figure 1 (right) shows the one-dimensional phase diagram for $\Omega = 4$, which closely resembles the one obtained using GA. Similar to the GA, we observe a pair superfluid phase, which for integer $\langle\hat{n}\rangle$ approaches all the way to the tip of the MI lobes. Away from the lobe tips we observe a direct MI-SF transition. Our one-dimensional results also confirm the absence of PSF for $\mathcal{J}_0(\Omega) > 0$.

The case $\mathcal{J}_0(\Omega) = 0$ is particularly interesting, since for neighboring sites i and j with equal number of particles, the process $|n\rangle_i|n\rangle_j \to |n\pm1\rangle_i|n\mp1\rangle_j$ is forbidden. However, the hopping $|n\pm1\rangle_i|n\rangle_j \to |n\rangle_i|n\pm1\rangle_j$ is still characterized by the usual rate J. This difference has a remarkable impact for both the MI and the SF phases.

For $J = 0$, the ground state of Eq. (4) is, as for the standard BHM ($\Omega = 0$), a defect-free MI $\bigotimes_j|n\rangle_j$ for $n - 1 < \mu/U_0 < n$ [28]. For $\Omega = 0$ and $J > 0$, this state is not an eigenstate of Eq. (4), and quantum fluctuations induce a finite particle-hole population in the Mott insulator with an associated nonlocal parity order [6]. Interestingly, the defect-free state remains an eigenstate of Eq. (4) for $\mathcal{J}_0(\Omega) = 0$. As a result, the whole MI lobe is characterized by the absence of particle-hole defects.

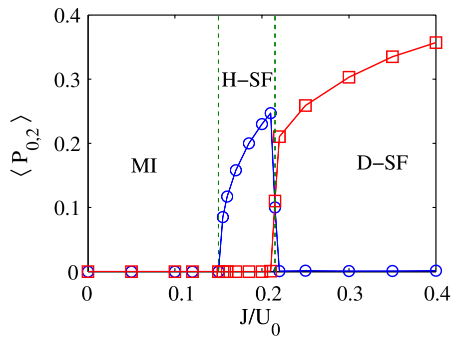

FIG. 2 (color online). iTEBD results for the holon (circles) and doublon (squares) populations as a function of J/U_0 for a one-dimensional system with $\mu/U_0 = 0.3$ and $\Omega = 2.405$. Note the absence of defects in the Mott insulator ($J/U_0 < 0.15$), and the appearance of the holon SF (H-SF) and doublon SF (D-SF).

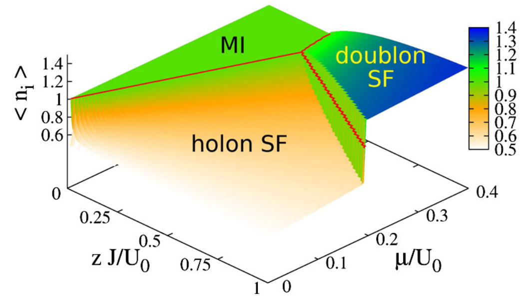

FIG. 3 (color online). Homogeneous GA results for $\langle \hat{n} \rangle$ as a function of J/U_0 and μ/U_0 for $\Omega = 2.405$. The solid red lines denote the boundary of the Mott insulator and the line of integer filling 1. Note the abrupt jump in the density at that line, indicating the transition between the holon SF and doublon SF regimes.

Although this is typically an artifact in the mean-field GA, in this case it is an exact result for any dimensions. This is illustrated for the one-dimensional case in Fig. 2, where our iTEBD results show a vanishing variance $(\Delta n)^2 = \langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2$ within the whole Mott insulator. A defect-free Mott insulator may be revealed by parity-order measurements using site-resolved techniques [6]. Whereas for the standard BHM doublon-hole pairs reduce parity order, a defect-free Mott insulator results in unit parity in the whole Mott phase.

Conversely, particles or holes ($|n \pm 1\rangle$) on top of the state $\bigotimes_j |n\rangle_j$ acquire also remarkable properties. For any Ω, extra particles and holes move with a hopping rate $(n+1)J$ and nJ, respectively. For $\Omega = 0$ defects are unstable, being created and destroyed by processes $|n\rangle_i |n\rangle_j \leftrightarrow |n \pm 1\rangle_i |n \mp 1\rangle_j$. Since these processes are forbidden for $\mathcal{J}_0(\Omega) = 0$, defects remain stable [29]. Neglecting occupations other than n and $n \pm 1$, the defects are described by an effective Hamiltonian $H_h + H_p$, where

$$H_h = -Jn \sum_{\langle i,j \rangle} h_i^\dagger h_j + (\mu - U_0(n-1)) \sum_i h_i^\dagger h_i, \qquad (5)$$

$$H_p = -J(n+1) \sum_{\langle i,j \rangle} p_i^\dagger p_j + (U_0 n - \mu) \sum_i p_i^\dagger p_i, \qquad (6)$$

characterize, respectively, the physics of holes and particles, with the hard-core assumption $p_i^\dagger p_i + h_i^\dagger h_i = 0$ or 1, with h_i (p_i) the operators for extra holes (particles) at site i. In Eqs. (5) and (6) we have set the energy of the defect-free MI state $E_{\rm MI} = 0$. Thus the system behaves as a two-component hard-core lattice Bose gas. For higher dimensions, a dilute gas of extra holes (holon gas) may be considered as a basically free (superfluid) Bose gas, with a dispersion $E_h(\mathbf{q}) = \mu - U_0(n-1) + n\epsilon_{\mathbf{q}}^0$, where $\epsilon_{\mathbf{q}}^0 = -2J\sum_{j=x,y,z} \cos(q_j d)$ for a three dimensional cubic lattice and d is the lattice spacing. On the other hand, the dilute gas of extra particles ("doublon" gas [30]) has a dispersion $E_p(\mathbf{q}) = U_0 n - \mu + (n+1)\epsilon_{\mathbf{q}}^0$.

At zero temperature, the defect gas condenses for $\mu < \mu_c \equiv U_0(n - 1/2) - Jz$ at the bottom of the holon band, $E_h(0)$, acquiring a pure holon character. On the other hand, for $\mu > \mu_c$ the system condenses at $E_p(0)$ into a pure doublon gas. Hence, remarkably, we expect an abrupt jump of $\langle \hat{n} \rangle$ (i.e., a diverging compressibility) at the line $\mu = \mu_c$, which coincides with the line of integer $\langle \hat{n} \rangle = n$. Figure 3 depicts our GA results for the density as a function of μ/U_0 and J/U_0, which, as expected from the previous discussion, presents an abrupt jump between a holon and a doublon superfluid.

In one dimension, the defects behave, due to the hard-core constraint, rather as a two-component Tonks gas, but a similar two-band reasoning applies, and we may also expect the existence of pure holon and doublon superfluids. Figure 2 shows our iTEBD results in the vicinity of $\langle \hat{n} \rangle = 1$ for the holon (doublon) populations $\langle \hat{P}_0 \rangle$ ($\langle \hat{P}_2 \rangle$), with $\hat{P}_n = \prod_{n' \neq n} (\hat{n} - n')/(n - n')$. In addition to the Mott insulator characterized by $\langle \hat{P}_{0,2} \rangle = 0$, we observe a holon SF ($\langle \hat{P}_2 \rangle = 0$) and an abrupt jump to a doublon SF ($\langle \hat{P}_0 \rangle = 0$). Note that a pure doublon SF or holon SF excludes PSF.

At constant μ for $\mathcal{J}_0(\Omega) = 0$ the system undergoes a MI-doublon (holon) SF transition at a critical tunneling $J_c(\mu)$ for which $E_{p(h)}(0) = E_{\rm MI}$. On the contrary, at constant integer $\langle \hat{n} \rangle$, there is no one-dimensional MI-SF transition at finite hopping J. Due to the absence of processes $|n\rangle_i |n\rangle_j \leftrightarrow |n \pm 1\rangle_i |n \mp 1\rangle_j$, doublons and holons cannot swap their positions through second-order superexchange. As a result, if holons and doublons coexist (which only happens at the singular integer filling line), superfluidity is absent. Our DMRG results for $\langle \hat{n} \rangle = 1$ confirm this insulating character for any J, showing a clear transition between a defect-free insulator and an insulator with a finite defect density.

For a finite but small $\mathcal{J}_0(\Omega)$, the SF regions retain to a large extent their holon and doublon character, although the concentration of doublons in the holon SF and holons in the doublon SF increases for growing $\mathcal{J}_0(\Omega)$ and J.

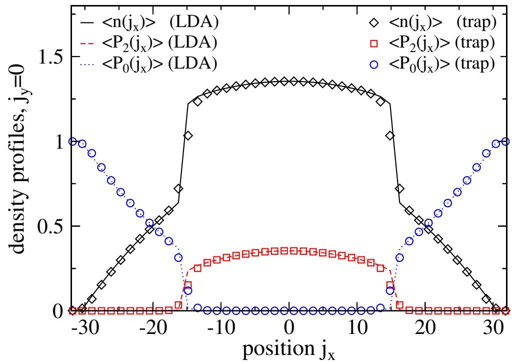

FIG. 4 (color online). GA results for the site densities $\langle \hat{n}_j \rangle$ and the on-site holon and doublon populations for a two-dimensional lattice with a harmonic confinement $V(j_x, j_y) = V_0(j_x^2 + j_y^2)$, with $V_0/J = 0.0075$, interaction $U_0/J = 5.33$, a central chemical potential $\mu_0/J = 3$, and $\Omega = 2.45$ ($\mathcal{J}_0(\Omega) \simeq 0$). Note the central doublon-SF region, surrounded by a holon-SF ring, and the abrupt density drop separating both regimes. Lines indicate local-density approximation (LDA) results.

The coexistence region for holons and doublons is hence not any more singular, although it remains characterized by a large compressibility for small $\mathcal{J}_0(\Omega)$. For $\mathcal{J}_0(\Omega) < 0$ this coexistence region becomes the pair superfluid phase discussed above. Away from the Mott tip a direct MI-SF transition is observed, as discussed above, since at the MI boundary holons and doublons do not coexist.

Let us finally discuss some experimental questions. Optimal experimental conditions for periodically modulated interactions are provided by ^{85}Rb, which has a particularly large $a_{bg} \simeq -400a_B$ (with a_B the Bohr radius), and a broad Feshbach resonance at $B_r = 155.2$ G, with a width $\Delta B = 11.6$ G [31]. The desired form $a(t) \approx a_0 + a_1 \cos(\omega t)$ can be achieved for a magnetic field dependence $B(t)/G \simeq 167.56 + 5.58 \cos(\omega t)$, with $a_0 \approx 20a_B$ and $a_1 \approx 200a_B$. We consider a lattice spacing $d = 0.5$ μm, and potential depth $V_L = sE_R$, where $E_R = \hbar^2\pi^2/2Md^2$ is the recoil energy. For $s \approx 17$ ($J \ll U_0$), the value $\Omega = 2.4$ ($\mathcal{J}_0(\Omega) \simeq 0$) is obtained for $\omega \simeq 2\pi \times 900$ Hz $\gg U_0/\hbar = 2\pi \times 217$ Hz, ensuring that only one Floquet manifold is relevant [32].

In order to address the question of detection, we have to consider the transformation [Eq. (2)] between the Floquet $|\{n_j\}, m\rangle$ and the Fock $|\{n_j\}\rangle$ basis. The densities $\langle \hat{n}_i \rangle$ are equivalent in both; therefore, the large compressibility regions characteristic of $|\mathcal{J}_0(\Omega)| \simeq 0$ may be revealed in *in situ* experiments with an additional harmonic confinement. This is illustrated in Fig. 4, where we show inhomogeneous GA results for a harmonic trap in two dimensions. As expected from the local-density approximation, we observe an abrupt density jump when the local chemical potential crosses its critical value.

Interpretation of other observables, as, e.g., the momentum distribution in time-of-flight (TOF) measurements, may be more involved, since $\langle\{n_j'\}|b_i^\dagger b_j|\{n_j\}\rangle \sim e^{-iV(t)(n_i-n_j+1)}\langle\{n_j'\}, m|b_i^\dagger b_j|\{n_j\}, m\rangle$. However, for the holon SF and doublon SF phases the TOF measurement is almost time-independent for small $|\mathcal{J}_0(\Omega)|$. Indeed this weak dependence is in itself a proof of the holon or doublon character of the SF. For large $|\mathcal{J}_0(\Omega)|$ the nonlinear conversion is an issue, and in general measurement results are periodic.

In summary, periodically modulated interactions lead to a rich physics for cold gases in optical lattices, characterized by a nonlinear hopping depending on the number difference at neighboring sites. This hopping can lead to pair superfluid phases, and also to defect-free Mott states, and holon and doublon superfluids, which may be revealed by parity measurements and by abrupt jumps of the *in situ* densities in harmonically trapped lattice gases.

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