Superfluid-Insulator Transition in a Periodically Driven Optical Lattice

André Eckardt, Christoph Weiss, and Martin Holthaus

Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg, Germany

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We demonstrate that the transition from a superfluid to a Mott insulator in the Bose-Hubbard model can be induced by an oscillating force through an effective renormalization of the tunneling matrix element. The mechanism involves adiabatic following of Floquet states, and can be tested experimentally with Bose-Einstein condensates in periodically driven optical lattices. Its extension from small to very large systems yields nontrivial information on the condensate dynamics.

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The Bose-Hubbard model plays an important role in condensed matter physics, since it embodies essential features of strongly interacting Bose systems in a minimal manner, namely, the competition between kinetic and potential energy effects, and the resulting quantum phase transition from a superfluid to a Mott insulator [1,2]. It describes Bose particles on a lattice with on-site interaction, so that particles occupying the same lattice site repel each other, while tunneling is allowed between adjacent sites. This is expressed by the Hamiltonian

$$\hat{H}_0 = -J\sum_{\langle i,j\rangle}(\hat{c}_i^\dagger\hat{c}_j + \hat{c}_j^\dagger\hat{c}_i) + \frac{U}{2}\sum_j \hat{n}_j(\hat{n}_j - 1), \quad (1)$$

where $\hat{c}_j^{(\dagger)}$ is an annihilation (creation) operator for a boson on the site labeled j, and $\hat{n}_j = \hat{c}_j^\dagger\hat{c}_j$ denotes the corresponding number operator. The first sum runs over all pairs of neighboring sites i and j, with the matrix element J quantifying the strength of the tunneling contact. Moreover, U is the repulsion energy contributed by one pair of bosons located on the same site. Therefore, the characteristic dimensionless parameter is the ratio U/J: When $U \ll J$, so that tunneling dominates, the ground state of the system describes a superfluid, whereas it has the properties of a Mott insulator when the interaction dominates, $U \gg J$. Mean-field theory [1,2] gives the critical value $(U/J)_c \approx z \times 5.83$ for the transition in a lattice filled with one particle per site, which captures the case of a three-dimensional (3D) cubic lattice with coordination number $z = 6$ reasonably well, whereas more refined methods [3] yield a Kosterlitz-Thouless transition with $(U/J)_c \approx 3.8$ for $d = 1$.

After the model (1) had long been of primarily theoretical interest, it has found its laboratory realization with Bose-Einstein condensates in optical lattices [4–6]. In such systems, the expected transition has been observed upon varying the lattice depth, both for $d = 3$ [7] and $d = 1$ [8]. In this Letter, we demonstrate that the transition from a superfluid to a Mott insulator can be induced in an altogether different manner which, in contrast to all scenarios studied before, hinges on the effect of a time-dependent force, and which can be assessed experimentally with condensates in periodically modulated optical lattices. We investigate a *periodically forced* Bose-Hubbard model for $d = 1$, as described by the explicitly time-dependent Hamiltonian

$$\hat{H}(t) = \hat{H}_0 + K\cos(\omega t)\sum_j j\hat{n}_j, \quad (2)$$

where the equidistant sites are labeled according to their position in ascending order. The oscillating term, which mimics a monochromatic electric dipole potential with frequency ω and amplitude K, can be realized experimentally by periodically shifting the position of a mirror employed to generate the standing laser wave, and transforming to the comoving frame of reference [9,10]. We argue that the driven system (2) behaves, for sufficiently high frequencies, similar to the undriven system (1), but with the tunneling matrix element J of the latter being replaced by the effective matrix element

$$J_{\rm eff} = J\,\mathcal{J}_0(K/(\hbar\omega)), \quad (3)$$

where $\mathcal{J}_0(x)$ denotes the ordinary Bessel function of order zero. Hence, the actual control parameter becomes $U/J_{\rm eff}$, which can be varied by adjusting the parameters of the periodic modulation. This implies the possibility to switch between the superfluid and the insulator state by changing, e.g., the modulation strength K.

The rescaling (3) is not unfamiliar with periodically driven single-particle quantum systems. It occurs, among others, when a particle moves on a periodically forced 1D lattice with nearest neighbor coupling [11,12], such as an electron in a semiconductor superlattice [13]. It also underlies the $\mathcal{J}_0$-type renormalization of atomic g factors in oscillating magnetic fields [14,15], and the coherent destruction of tunneling of a particle in a periodically forced double well [16,17]. However, as is discussed below, the many-body system (2) is significantly more involved when the thermodynamic limit is taken; the rescaling (3) then describes only part of the relevant physics.

Our analysis is based on quantum Floquet theory [18]: Since the Hamiltonian (2) depends periodically on time, $\hat{H}(t) = \hat{H}(t + T)$ with period $T = 2\pi/\omega$, there exists a complete set of solutions to the time-dependent many-body Schrödinger equation of the form $|\psi_n(t)\rangle = |u_n(t)\rangle \times \exp(-i\varepsilon_n t/\hbar)$, where the Floquet functions $|u_n(t)\rangle$ inherit the period of the driving force, satisfying $|u_n(t)\rangle = |u_n(t+T)\rangle$. Thus, Floquet states for periodically time-dependent quantum systems, obtained by solving the eigenvalue equation

$$[\hat{H}(t) - i\hbar\partial_t]|u_n(t)\rangle = \varepsilon_n|u_n(t)\rangle, \tag{4}$$

constitute an analog of Bloch states known from spatially periodic crystals; the eigenvalues ε_n, which describe the time evolution of these states in close analogy to the evolution of energy eigenstates, are called quasienergies. While in solid-state physics quasimomenta are defined up to an integer multiple of a reciprocal lattice vector, quasienergies are defined up to an integer multiple of $\hbar\omega$: If $|u_n(t)\rangle$ solves Eq. (4) with eigenvalue ε_n, and $m = 0, \pm1, \pm2, \ldots$, then $|u_n(t)\rangle\exp(im\omega t)$ is a T-periodic eigensolution with quasienergy $\varepsilon_n + m\hbar\omega$. The quasienergy spectrum of a periodically time-dependent quantum system thus possesses a Brillouin zonelike structure, the width of one zone being $\hbar\omega$.

We then employ the Floquet basis

$$|\{n_j\}, m\rangle = |\{n_j\}\rangle\exp\left[-i\frac{K}{\hbar\omega}\sin(\omega t)\sum_j jn_j + im\omega t\right], \tag{5}$$

where $|\{n_j\}\rangle$ indicates a Fock state with n_j particles on the jth site, and m again accounts for the zone structure. The eigenvalue problem (4) refers to an extended Hilbert space of T-periodic functions, in which the time variable is regarded as a coordinate [19], so that the scalar product in that space is given by

$$\langle\langle\cdot|\cdot\rangle\rangle = \frac{1}{T}\int_0^T dt\langle\cdot|\cdot\rangle, \tag{6}$$

i.e., by the usual scalar product $\langle\cdot|\cdot\rangle$ combined with time-averaging. Hence, the quasienergies are obtained by computing the matrix elements of the operator $\hat{H}(t) - i\hbar\partial_t$ in the basis (5) with respect to the scalar product (6), and diagonalizing. Denoting the Hamiltonian $\hat{H}_0$ with $J = 0$, which is diagonal in the basis (5), by $\hat{H}_{\rm int}$, and its J-proportional tunneling term by $\hat{H}_{\rm tun}$, we find

$$\langle\langle\{n_j'\}, m'|\hat{H}(t) - i\hbar\partial_t|\{n_j\}, m\rangle\rangle = \delta_{m',m}[\langle\{n_j'\}|\hat{H}_{\rm int}|\{n_j\}\rangle + m\hbar\omega] + s^{m'-m}\mathcal{J}_{m'-m}(K/(\hbar\omega))\langle\{n_j'\}|\hat{H}_{\rm tun}|\{n_j\}\rangle, \tag{7}$$

where $s = \sum_j(n_j' - n_j)j = \pm1$, since $\hat{H}_{\rm tun}$ transfers only one particle by one site. We observe that with respect to the "photon" index m this matrix has a transparent block structure: The diagonal blocks with $m = m'$ reproduce the matrix that yields the eigenvalues of the undriven system, but with J replaced by $J_{\rm eff}$ according to Eq. (3), and replicas shifted by integer multiples of $\hbar\omega$. These blocks are coupled by nondiagonal ones proportional to Bessel functions $\mathcal{J}_{m'-m}(K/(\hbar\omega))$. Obviously, the anticipated rescaling (3) holds only to the extent that these couplings can be neglected. This will be the case, at least in a perturbative sense, if the block separation $\hbar\omega$ is much larger than both the energy scale J of the coupling and the energy scale U associated with the diagonal blocks, i.e., for high frequencies $\hbar\omega \gg \max\{J, U\}$.

To demonstrate that this reasoning is justified, we present numerical results for small systems. Figure 1 depicts the exact energy spectrum for a one-dimensional undriven model (1) with $N = 5$ particles on $M = 5$ sites. Even here, the precursor of the superfluid-insulator transition already is apparent: With increasing U/J the system's ground state, associated with a uniform distribution of the particles over the sites, splits off from the group of excited states, which describe various patterns of particle-hole excitations. In the limit of an infinitely large system, $N \to \infty$ and $M \to \infty$ with $N/M = 1$ held constant, the excited states form continuous energy bands; the ground state then splits off from the lowest band at a finite $(U/J)_c$ [3]. This separation of an individual state from the continuum indicates the transition to the Mott insulator state.

For comparison, Fig. 2 shows the first Brillouin zone of numerically computed quasienergies for the driven system (2), again with $N = M = 5$, scaled frequency $\hbar\omega/J = 14$, and scaled driving amplitude $K/\hbar\omega = 1.5$. Since $\mathcal{J}_0(1.5) \approx 0.5$, this set of parameters allows for a convenient test of the hypothesis (3): With $J_{\rm eff} \approx J/2$, the *quasienergy* spectrum of the driven system (2) for a given parameter U/J should correspond (apart from its zone structure) to the *energy* spectrum of the undriven system (1) with the same $U/J_{\rm eff}$, which is about $2U/J$. This is

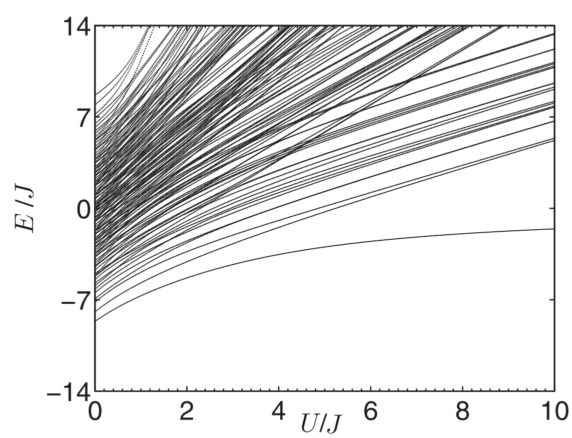

FIG. 1. Exact energy spectrum of a small one-dimensional undriven lattice (1) with $M = 5$ sites and $N = 5$ particles versus Mott-Hubbard parameter U/J. The splitting off of the ground state with increasing interaction strength can be regarded as a precursor of the quantum phase transition.

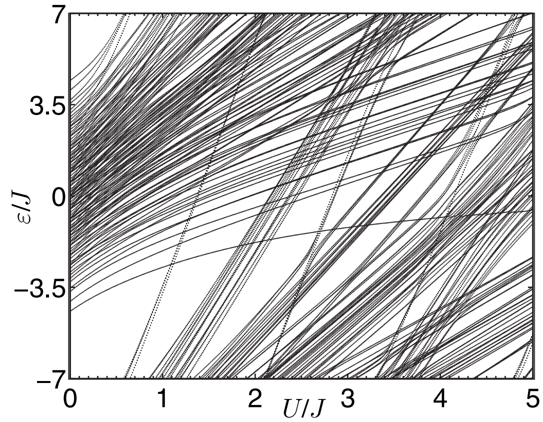

FIG. 2. First Brillouin zone of the exact quasienergy spectrum of the driven 1D system (2) with $N = M = 5$, $\hbar\omega/J = 14$, and $K/\hbar\omega = 1.5$. This spectrum is recovered approximately from the energy eigenvalues shown in Fig. 1, if J is replaced by $J_{\rm eff} \approx J/2$ here, and the energies are taken modulo $\hbar\omega$.

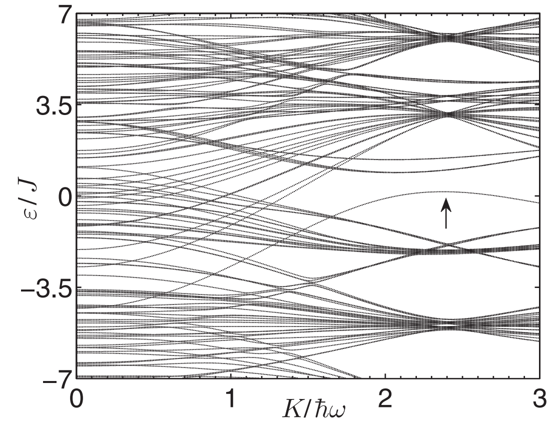

FIG. 3. First Brillouin zone of the exact quasienergy spectrum of the driven 1D system with $N = M = 5$, $\hbar\omega/J = 14$, and $U/J = 3$ versus scaled driving amplitude $K/\hbar\omega$. For $K/\hbar\omega \approx 2.4$, close to the first zero of $\mathcal{J}_0$, the tunneling contact is (almost) switched off, resulting in a collapse of the different bands. In the vicinity of this value, the Floquet state evolving from the system's ground state (marked by the arrow) has the properties of a Mott insulator, even though the undriven system's ground state is superfluid for $U/J = 3$.

borne out, to remarkable accuracy, by a comparison of Figs. 1 and 2: With the scales of the respective axes differing by a factor of 2, the eigenvalues plotted in Fig. 2 almost equal those in Fig. 1. As a consequence of the Brillouin zone structure, quasienergy eigenvalues that disappear at the upper zone boundary reappear again at the lower one. This reappearance is a source of substantial complications: States originating from different Brillouin zones are coupled through the matrix elements neglected in the explanation of the renormalization (3), so that many apparent level crossings in Fig. 2 actually are tiny avoided crossings. It is the high-frequency condition $\hbar\omega \gg \max\{J, U\}$ which guarantees that these avoided crossings remain too narrow to be resolved. If this condition is not met, a multitude of large avoided crossings appears in the spectrum, thus revealing typical signatures of quantum chaos [20].

Figure 3 shows quasienergies for $U/J = 3$ kept fixed, again for $\hbar\omega/J = 14$, as functions of the scaled amplitude $K/(\hbar\omega)$. For $K/(\hbar\omega) \approx 2.4$, close to the first zero of $\mathcal{J}_0$, the tunneling contact is quenched almost entirely, so that the various bands of particle-hole excitations collapse. In the vicinity of this point, the Floquet state evolving from the unperturbed ground state must have the properties of a Mott insulator, although the ground state of the undriven system describes a superfluid for $U/J = 3$.

To verify this conclusion, we have solved the time-dependent Schrödinger equation for a system with $N = M = 7$ and $U/J = 3$, initially prepared in its superfluid ground state and then subjected to periodic forcing with frequency $\hbar\omega/J = 14$, and an amplitude $K/(\hbar\omega)$ which increases linearly from 0 to 2.4 during the first 100 cycles T, then stays constant for another 100 cycles, and finally is linearly ramped down to zero between $t = 200T$ and $t = 300T$. Experimentally, the superfluid phase is detected by a sharply peaked reciprocal lattice pattern in the momentum distribution, $\varrho(p) = \sum_{j,k}\langle c_j^\dagger c_k\rangle e^{-ip(j-k)}$, which can be measured by time-of-flight absorption imaging. (Here, p is given in multiples of $\hbar$/lattice constant.) Figure 4 depicts our result: Since Floquet states respect an approximate adiabatic principle [21], the initial superfluid ground state is first adiabatically transformed into a Mott insulator state,

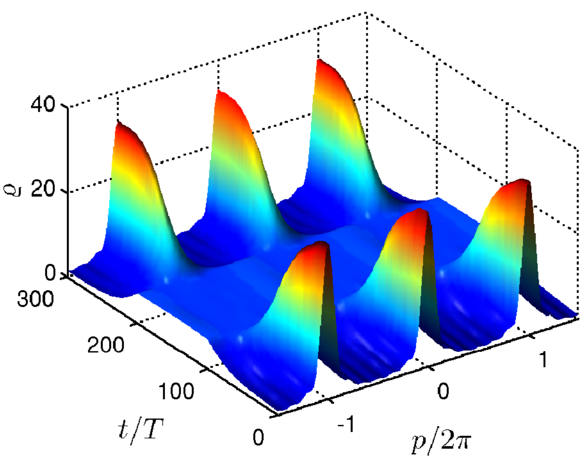

FIG. 4 (color online). Time evolution of the momentum distribution $\varrho(p)$ obtained by solving the time-dependent Schrödinger equation for $N = M = 7$, $\hbar\omega/J = 14$, and a slowly varying amplitude $K/(\hbar\omega)$, which is linearly ramped up to 2.4 during the first 100 cycles T, then stays constant for another $100T$, and is ramped down to zero during the final 100 cycles. The system was initially in its ground state; the distribution was recorded at integer multiples of T. The disappearance and reappearance of the peak pattern signals the transition from the superfluid to the Mott state and back.

as witnessed by the disappearance of the peaked momentum distribution, and then transformed back to the initial state, apart from a remaining excitation of other states totaling a few percent. This is a major result: The amplitude of the periodic force decides whether the system is superfluid or in a Mott insulator state.

When extrapolating from these model calculations to large systems, two issues have to be considered. First, when increasing the number of lattice sites while maintaining an occupancy of one particle per site, say, the quasienergy levels fill the Brillouin zone densely; in the thermodynamic limit, the spectrum probably is a continuum. Then there is no ''sharp'' Floquet state evolving from the ground state, but rather a resonance with a finite lifetime, due to the residual couplings to other states. Starting from an undriven, infinite system with a superfluid ground state, and switching on the periodic force, we conjecture that a Mott-insulator-like resonance appears at that amplitude K which, after rescaling according to Eq. (3), corresponds to that tunneling matrix element J which marks the quantum phase transition in the undriven system. Second, for an infinitely large lattice there is no adiabatic limit when switching on the driving force [22]; turn-on and turn-off necessarily have to take place within a short interval. Our calculations indicate that adiabatic following can even be improved by *shortening* the turn-on time, since Landau-Zener transitions at narrow avoided crossings, possibly corresponding to condensate heating, then are suppressed.

While these issues are still not covered by rigorous mathematical theorems on periodically driven quantum systems [23], and remain out of reach of even the most powerful supercomputers, they can be addressed in the laboratory. In experiments with cold atoms in driven optical lattices [10], narrowing of Bloch bands compatible with the rescaling (3) has already been observed, even though the single-band regime has not been reached. Employing Bose-Einstein condensates in optical lattices in order to realize the driven Bose-Hubbard model (2), one has to respect not only the high-frequency condition $\hbar\omega > \max\{J, U\}$ required for the approximate Bessel-function rescaling (3), but there is the obvious additional condition $\hbar\omega < \Delta$, where Δ denotes the gap between the lowest two Bloch bands of the undriven lattice, in order to exclude transitions to higher band states. Elementary estimates in the spirit of Ref. [5] suggest that under typical conditions (as provided by ^{87}Rb atoms in a lattice created by laser radiation of $\lambda = 852$ nm wavelength [7]) this leaves a viable window of frequencies in the low kHz regime. For higher filling factors, or in 3D lattices with forcing in all three directions, the critical parameter $(U/J)_c$ becomes much larger, allowing one to employ deeper lattices with larger band gap Δ, and hence to work with still higher frequencies without violating the single-band approximation. A quantity of key interest in such experiments will be the extent to which, after starting from a superfluid ground state, then ramping up the force into the insulator regime and ramping it down again as in Fig. 4, the superfluid peak pattern reappears, providing information on both the lifetime of the conjectured Mott-like resonance state and the degree of adiabatic following, or, more generally, on the extent to which the quantum evolution of a mesoscopic matter wave can be guided even under critical conditions. Thus, the scenario envisioned here is not intended as a look at the common superfluid-insulator transition from a different angle, but aims at obtaining genuinely new, nontrivial information on condensate dynamics.

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