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First-Order Phase Transitions in Optical Lattices with Tunable Three-Body Onsite Interaction

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We study the two-dimensional Bose-Hubbard model in the presence of a three-body interaction term, both at a mean-field level and via quantum Monte Carlo simulations. The three-body term is tuned by coupling the triply occupied states to a trapped universal trimer. We find that, for a sufficiently attractive three-body interaction, the $n = 2$ Mott lobe disappears and the system displays first-order phase transitions separating the $n = 1$ from the $n = 3$ lobes and the $n = 1$ and $n = 3$ Mott insulator from the superfluid. We also analyze the effect of finite temperature and find that transitions are still of first order at temperatures $T \sim J$, where J is the hopping matrix element.

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The Bose-Hubbard (BH) model and its second-order superfluid (SF) Mott-insulator (MI) transition represent one of the paradigmatic examples of strongly interacting many-body physics in lattice structures [1]. The unprecedented control over ultracold atoms in optical lattices allows for not only a clean experimental realization of the BH model [2,3] but also the exploration of a panoply of quantum effects beyond the standard BH model (see Refs. [4–12]).

One key element for such impressive progress is the possibility of tuning two-body interactions by using Feshbach resonances or changing the strength of the lattice confinement. More recently, effective multibody interactions have been experimentally observed [13,14]. The question that naturally arises is how these interactions affect the many-body behavior. Topological phases such as fractional quantum Hall states appear as ground states to model Hamiltonians with strong three-body interactions while exotic quantum phases have been predicted for bosonic Hamiltonians with many-body interactions, such as the ring exchange model [15,16]. An important first step in realizing these models using ultracold atoms was the recognition that strong three-body losses lead to an effective hard-core three-body interaction that can be used, for instance, to stabilize the BH model with attractive two-body interactions [17]. Under these conditions, the system can undergo a *first-order* MI-to-SF transition in the presence of strong pairing interactions [18]. Despite these recent studies, lattice systems with three-body interactions remain largely unexplored.

In this Letter, we analyze how the many-body physics of the BH model is affected by the presence of local and tunable three-body interactions. First, we propose a mechanism for engineering a three-body on-site interaction term, U_3 , which is controlled by an external rf pulse that couples the triply occupied state with a three-body bound state associated with an excited hyperfine state. This local three-body interaction

only affects triply occupied sites leading to a modified BH Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} a_i^\dagger a_j + \sum_i \left[\frac{U}{2} n_i(n_i - 1) + \delta_{n_i,3} U_3 - \mu n_i \right], \quad (1)$$

where a_i^\dagger (a_i) is the bosonic creation (annihilation) operator, $n_i = a_i^\dagger a_i$, J is the hopping matrix element, U is the two-body on-site interaction, U_3 is the three-body on-site interaction, μ is the chemical potential, and $\langle i, j \rangle$ denotes summation over nearest-neighbor sites only [see Fig. 1(a)]. Note that the three-body interaction considered here is different from the more conventional interaction of the form $U_3 n(n-1)(n-2)/6$.

Next, we use a mean-field Gutzwiller approach to study the BH Hamiltonian in the presence of such three-body interaction in the $U > 0$, $U_3 < 0$ regime. We focus on the $|U_3| > U$ region where the $n = 2$ ($n = 4$) lobe disappears. In this regime, a direct first-order phase transition at finite hopping can occur between the $n = 1$ and $n = 3$ lobes. Quantum Monte Carlo (QMC) simulations [19] confirm the existence of a first-order phase transition and provide quantitative predictions of the phase diagram in two dimensions and particular values of U and U_3 . Finally, we briefly discuss finite temperature effects and experimental signature of the first-order transition.

To achieve a separately tunable, on-site, three-body interaction of the form shown in Eq. (1), we envision a system in which a universal three-body bound state is attached to an excited hyperfine threshold [20] which is coupled to the identical boson ground state by an external rf field [shown schematically in Fig. 1(b)] [21,22]. In this scheme, identical bosons in two different hyperfine states (labeled b and x for the lowest state and an excited state, respectively) sit on a single site which we model as an isotropic oscillator with

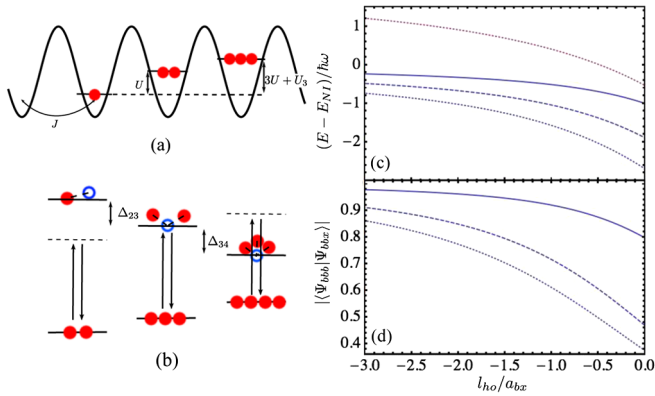


FIG. 1 (color online). Schematic representations of (a) the Bose-Hubbard Hamiltonian considered here [Eq. (1)] and (b) the rf field-tuned three-body on-site interaction are shown. In (b), the red and open, blue circles represent bosons in the lowest and (excited) hyperfine states (b and x), respectively. The dotted line represents the energy the rf field is tuned to with respect to the excited two- and four-body states. (c) The energy of the lowest two-, three-, and four-body states (solid, dashed, and dotted lines, respectively) in the excited hyperfine state is shown in trap units with respect to the noninteracting energy E_{NI} . Also shown is the energy of the first excited four-body state (upper dotted line) to demonstrate that the universal three-body state is in fact isolated. (d) The wave-function overlap between the noninteracting ground state and the lowest excited hyperfine state is shown as a function of l_{ho}/a_{bx} for two, three, and four atoms (solid, dashed, and dotted lines, respectively). In both (c) and (d), the calculations are done for model Rb atoms described in the text.

oscillator frequency ω and length l_{ho} . For a three-body bound state to form in an excited hyperfine state, we consider a system with a repulsive bb nonresonant interaction ($0 < a_{bb} \ll l_{ho}$) and a large bx scattering length ($a_{bb} \ll |a_{bx}|$). In this situation, universal three-body Efimov states form attached to the bbx three-body hyperfine state [20].

To analyze this scenario, we explore two-, three-, and four-body single-site physics within the harmonic approximation, using model short-range interactions and a correlated Gaussian basis set expansion [23,24]. We tune the interaction parameters to achieve a bbx Efimov trimer whose binding energy ($E_b = E_{NI} - E$ where E_{NI} is the noninteracting energy of the trapped system) is comparable to the trapping energy $\hbar\omega$ [see Fig. 1(c)]. This particular scenario is suitable for achieving the proposed Hamiltonian for two reasons. First, the two-, three-, and four-body binding energies are well separated, allowing the rf pulse to be tuned in resonance with a particular single-site occupancy; second, the large wave-function overlaps [see Fig. 1(d)] imply an efficient rf transition probability. Our numerical calculations show that the lowest three-body energy in the bbx configuration is lower than the two-body energy (bx configuration), and that, for each Efimov trimer state, there is a single four-body state ($bbbx$ configuration) bound below the trimer state. All other four-body states lie above

the trimer energy. This is in contrast to the more commonly considered case of four identical bosons in free space in which there are both a deeply bound and a weakly bound tetramer associated with each Efimov state [25]. The energies for two-, three-, and four-body states are shown schematically in Fig. 1(b) along with the energies at which the rf field is tuned to (dotted lines).

By detuning the rf field to the red of the Efimov state for three-body occupation, both the two- and three-body identical boson ground states are shifted down. However, because there is an energy difference between the two- and three-body transitions, the two-boson state is shifted significantly less than the three-body state. For higher occupation numbers, the rf field is far blue-detuned from the bound states, and thus the ground states with four or more identical bosons experience a weak upward shift. One might expect an additional shift in the states with higher occupation numbers (four or more), resulting from a three-boson, spectator particle-like system. However, for these weakly bound universal Efimov states, the size of the three-body state is similar to the trapping length, and thus additional bosons on site interact with the Efimov state and shift the resulting N -body excited state energy off resonance with the rf field.

As an initial study, we consider ^{85}Rb . Since the resonance structure for scattering between hyperfine states is not known, we will assume that there exists an s -wave scattering resonance between the lowest and first excited hyperfine states at some external magnetic field strength. For simplicity, we consider that identical bosons are roughly noninteracting. Assuming that the energy of the Efimov state is determined by the van der Waals length of Rb, $r_{vd} \approx 82$ a.u. [20], and a lattice site trapping frequency of $\omega = 2\pi \times 10$ kHz, an Efimov state will arise at $E_{3B} \approx -2\hbar\omega$ with respect to the bbx noninteracting energy. Under these circumstances, we predict that U_3 can be tuned to be attractive and of order U with a detuning of $\Delta \sim 1000$ kHz from the Efimov state transition energy. This large detuning also serves to mitigate the generally short lifetimes of Efimov states (on the order of $10 \mu\text{s}$ [26]).

This initial investigation, presented above as a plausibility argument, indicates that using the above scheme is feasible with existing experimental techniques. A more detailed study to determine the effects of rf coupling to an excited three-body state is left for future investigations [27]. Additionally, direct rf association of universal trimer states has already been demonstrated in ultracold, three-component Fermi and Bose gases [21], lending credibility to the experimental accessibility of this model.

We will now use Gutzwiller mean-field theory to study the modified BH Hamiltonian described by Eq. (1). The Gutzwiller mean-field theory is constructed by replacing the full Hamiltonian by an effective local Hamiltonian subject to a self-consistency condition. We introduce the

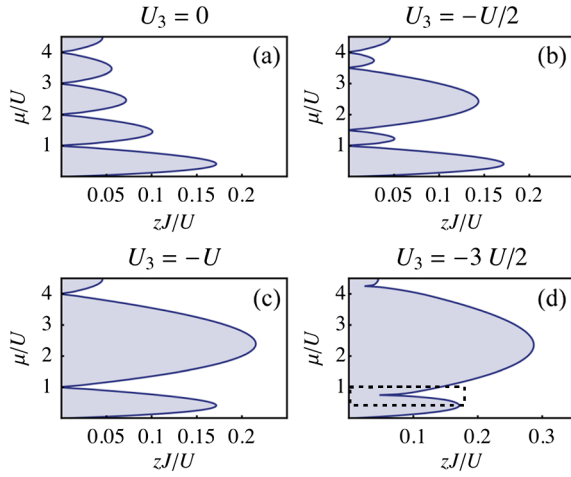


FIG. 2 (color online). Mean-field phase diagrams in the μ/U vs zJ/U plane, where $z = 4$ is the number of nearest neighbors in two dimensions, for $|U_3| = 0$ (a), $|U_3| = -U/2$ (b), $|U_3| = -U$ (c), and $|U_3| = -3U/2$ (d), are shown. When $0 < |U_3| < U$, the $n = 2$ and $n = 4$ lobes visibly shrink in favor of the $n = 3$ lobe, until they completely disappear at $|U_3| = U$ (c). For $|U_3| > U$, the $n = 3$ lobe begins to overlap with the $n = 1$ and $n = 4$ lobes, and a direct phase transition between MI lobes becomes possible. The dotted rectangle in (d) highlights the region examined in detail in Fig. 3.

superfluid order parameter $\psi = \langle a_i^\dagger \rangle = \langle a_i \rangle$ and the Gutzwiller wave function $|G\rangle = \prod_{i=0}^N (\sum_{n=0}^{\infty} f_n^{(i)} |n_i\rangle)$, so that the effective Hamiltonian for a translationally invariant system, i.e., $f_n^{(i)} = f_n$, takes the form

$$E[\psi] = -Jz\psi \sum_n \sqrt{n+1} (f_{n+1}^* f_n + \text{c.c.}) + zJ\psi^2 + E_n, \quad (2)$$

where z is the coordination number, f_n are variational parameters, and $E_n = \frac{U}{2}n(n-1) + \delta_{n,3}U_3 - \mu n$. The problem is now reduced to determining the set of coefficients $\{f_n\}$ which minimize $E[\psi]$ and satisfy the normalization condition $\langle G|G\rangle = \sum_n |f_n|^2 = 1$ [2,28,29].

Figure 2 shows the ground-state phase diagram of model (1) at different values of U_3 . As we increase the magnitude of $|U_3|$ from 0 to U , the $n = 2$ and $n = 4$ Mott lobes shrink considerably while the $n = 3$ lobe increases in size [as seen in Fig. 2(b)]. In particular, for $U_3 \leq -U$ the $n = 2$ and $n = 4$ lobes completely disappear since it is now energetically more favorable to have occupation number $n = 3$ [Fig. 2(c)]. This can be easily understood in the zero hopping limit. At $\mu = \mu_{12} = U$, a doubly occupied site has the same energy as a singly occupied one. At $\mu = \mu_{13} = (3U + U_3)/2$, instead, a singly occupied site has the same energy as a triply occupied one. The condition $\mu_{13} \leq \mu_{12}$ sets the U_3 value for which the second lobe disappears, i.e., $|U_3| > U$ (at $|U_3| = U$, sites with occupation number $n = 1, 2, 3$ are degenerate in energy for $\mu = \mu_{12} = \mu_{13}$). Direct transitions from MI occupation

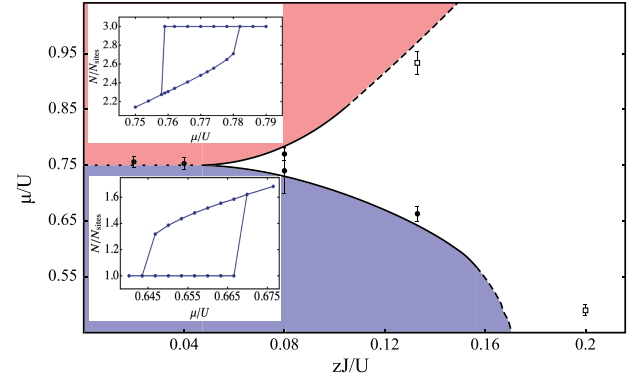


FIG. 3 (color online). First-order phase transitions at $U_3 = -1.5U$. The dotted line corresponds to the first-order phase transition from the $n = 1$ MI (lower blue) to $n = 3$ MI (upper pink) predicted by mean-field theory. Solid lines refer to mean-field first-order transitions from MI to SF. Solid circles are QMC results from hysteric curves. Dashed lines correspond to second-order mean-field MI-SF transitions. Open squares are second-order transition points from QMC. Lower (upper) inset shows examples of hysteric behavior for the $n = 1$ ($n = 3$) MI-to-SF transition.

numbers $n = 1$ to $n = 3$ survive at finite hopping [Fig. 2(d)], as confirmed below using QMC calculations. The same argument shows that $|U_3| > U$ also implies the disappearance of the 4th lobe. One can easily see that, upon further increasing U_3 , all lobes other than $n = 3$ will eventually disappear (e.g., at $U_3 = -3U$, the $n = 1$ and $n = 5$ lobes disappear).

We have monitored the behavior of mean-field energy [Eq. (2)] at fixed μ/U while varying J/U to study the order of phase transitions described by model (1). The formation of double minima structure in the mean-field energy functional $E[\psi]$ is a signature of first-order phase transitions. We have observed such double minima structures at $U_3 = -1.5U$ for the $n = 1$ MI-SF and $n = 3$ MI-SF transitions. The occurrence of first-order transitions can be understood with a simple argument. At fixed small J/U , $|U_3| \sim U$, and upon increasing (decreasing) μ in order to dope the $n = 1$ ($n = 3$) MI with particles (holes), double occupancy will be suppressed in favor of triply occupied sites. At a large enough $|U_3|$, such a mechanism will eventually prevent a gradual addition (subtraction) of particles resulting in first- rather than second-order transitions. Second-order transitions will be restored at a large enough J/U as the kinetic energy gain due to hopping of extra particles (holes) will again favor a gradual change in density.

In order to confirm the mean-field predictions, we have performed QMC simulations on a square lattice of linear size up to $L = 24$ (and $L = 30$ in certain cases) for selected values of J/U , and at $\beta = \frac{1}{k_B T} = L/J$, which corresponds to an effective zero-temperature regime. Figure 3 compares the QMC results with the mean-field predictions of the phase diagram for $U_3 = -3U/2$. As mentioned above, a direct transition from $n = 1$ MI (lower lobe) to $n = 3$ MI

(upper lobe) survives at finite hopping. This first-order transition is depicted by the dotted line, while the solid lines refer to first-order transitions from MI to SF. The solid and open symbols correspond to QMC predictions of the phase boundary with first- and second-order phase transitions.

To extract transition points, we have analyzed the particle density n as a function of μ . Additionally, we have performed hysteresis analysis by sweeping back and fourth in chemical potential and calculating the corresponding particle density. The hysteretic behavior of the system along the phase boundaries (solid symbols) further confirms that these are first-order transitions. We show two examples of such curves for the $n = 1$ MI-SF and $n = 3$ MI-SF transitions in the lower and upper inset, respectively. Based on the energy argument previously discussed, we expect the phase transition to become second order as J/U is increased. Indeed, larger kinetic energy will favor formation of particle or hole excitations on top of the MI. The energy gain due to hopping of the latter will compete with the attractive three-body interaction and will eventually restore the second-order MI-SF transition driven by addition or subtraction of a small number of particles from the MI regime.

We have used QMC simulations to benchmark the J/U values at which first-order phase transitions become second order. Second-order MI-SF transitions are depicted in Fig. 3 by dashed mean-field lines, with open squares representing QMC results. For $z = 4$, the $n = 1$ ($n = 3$) MI-SF transition becomes of second order at $zJ/U = 0.20 \pm 0.02$ ($zJ/U = 0.133 \pm 0.02$). We estimate the position triple point, using mean-field approximation [Eq. (2)], where we truncate the Hilbert space to the $n_i = 1, 2, 3$ states. Using this approximation, we find $(\frac{zJ}{U})_{TP} = -(U + U_3)/10$. For $U_3 = -1.5U$ and $z = 4$, this gives $J/U = 0.05$.

First-order phase transitions present in our model can be experimentally detected due to a loss of adiabaticity across the phase boundary even upon an arbitrarily slow ramping up or down of the optical lattice, as suggested in Ref. [30], or by observing hysteretic behavior. In addition, first-order phase transitions are characterized by discontinuity in density profiles, a local observable easily accessible with state-of-the-art techniques [31].

Finally, we have looked at how first-order phase transitions are affected by finite temperature. Strictly speaking, the MI state exists only at zero temperature. In practice, MI features persist up to temperature $T \sim 0.2U$ [32]. QMC results show that phase transitions are still of first order at temperatures of $T \sim J$, where MI features are still well defined. A more extensive study of the behavior of the system at finite temperatures will be the subject of future investigations.

Concluding, we have studied an extended version of the Bose-Hubbard model, which includes an attractive three-body interaction term U_3 , both at a mean-field level and by means of quantum Monte Carlo simulations. The three-body

term results from a universal three-body bound state attached to an excited threshold and can be tuned via an external rf field. We have found that, at $|U_3| > U$, where the $n = 2$ lobe disappears, there exists a first-order phase transition separating the $n = 1$ from the $n = 3$ lobes, which extend up to a triple point. A strong three-body attraction also affects the order of the MI-SF transition. We have found first-order transitions separating the $n = 1$ and $n = 3$ MI from the SF. We have also analyzed the effect of finite temperatures and found that transitions are still of first order at temperatures $T \sim J$.

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- [1] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, *Phys. Rev. B* **40**, 546 (1989).
- [2] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, *Phys. Rev. Lett.* **81**, 3108 (1998).
- [3] I. Bloch, J. Dalibard, and W. Zwerger, *Rev. Mod. Phys.* **80**, 885 (2008).
- [4] M. Pasiński, D. McKay, M. White, and B. DeMarco, *Nature Phys.* **6**, 677 (2010).
- [5] B. Gadway, D. Pertot, R. Reimann, and D. Schneble, *Phys. Rev. Lett.* **105**, 045303 (2010).
- [6] S. Ospelkaus, C. Ospelkaus, O. Wille, M. Succo, P. Ernst, K. Sengstock, and K. Bongs, *Phys. Rev. Lett.* **96**, 180403 (2006).
- [7] K. Günter, T. Stoferle, H. Moritz, M. Kohl, and T. Esslinger, *Phys. Rev. Lett.* **96**, 180402 (2006).
- [8] V. Gurarie, L. Pollet, N. V. Prokof'ev, B. V. Svistunov, and M. Troyer, *Phys. Rev. B* **80**, 214519 (2009).
- [9] F. Lin, E. S. Sørensen, and D. M. Ceperley, *Phys. Rev. B* **84**, 094507 (2011).
- [10] A. B. Kuklov and B. V. Svistunov, *Phys. Rev. Lett.* **90**, 100401 (2003).
- [11] Ş. G. Söyler, B. Capogrosso-Sansone, N. V. Prokof'ev, and B. V. Svistunov, *New J. Phys.* **11**, 073036 (2009).
- [12] T. Sowiński, *Phys. Rev. A* **85**, 065601 (2012).
- [13] S. Will, T. Best, U. Schneider, L. Hackermüller, D.-S. Lühmann, and I. Bloch, *Nature (London)* **465**, 197 (2010).
- [14] M. J. Mark, E. Haller, K. Lauber, J. G. Danz, A. J. Daley, and H.-C. Näger, *Phys. Rev. Lett.* **107**, 175301 (2011).
- [15] N. R. Cooper, *Phys. Rev. Lett.* **92**, 220405 (2004).
- [16] O. I. Motrunich and T. Senthil, *Phys. Rev. Lett.* **89**, 277004 (2002).
- [17] A. M. Daley, J. M. Taylor, S. Diehl, M. Baranov, and P. Zoller, *Phys. Rev. Lett.* **102**, 040402 (2009).
- [18] A. Kuklov, N. Prokofev, and B. Svistunov, *Phys. Rev. Lett.* **92**, 050402 (2004).

- [19] N. V. Prokof'ev, B. V. Svistunov, and I. S. Tupiysyn, *Phys. Lett. A* **238**, 253 (1998); *Sov. Phys. JETP* **87**, 310 (1998).
- [20] V. N. Efimov, *Phys. Lett. B* **33**, 563 (1970); E. Braaten and H. W. Hammer, *Phys. Rep.* **428**, 259 (2006); C. H. Greene, *Phys. Today* **63**, No. 3, 40 (2010); E. Nielsen and J. H. Macek, *Phys. Rev. Lett.* **83**, 1566 (1999); E. Nielsen, D. V. Fedorov, A. S. Jensen, and E. Garrido, *Phys. Rep.* **347**, 373 (2001).
- [21] T. Lompe, T. B. Ottenstein, F. Serwane, A. N. Wenz, G. Zürn, and S. Jochim, *Science* **330**, 940 (2010); S. Nakajima, M. Horikoshi, T. Mukaiyama, P. Naidon, and M. Ueda, *Phys. Rev. Lett.* **106**, 143201 (2011); O. Machtey, Z. Shotan, N. Gross, and L. Khaykovich, [arXiv:1201.2396v1](https://arxiv.org/abs/1201.2396v1).
- [22] T. Tscherbul and S. T. Rittenhouse, *Phys. Rev. A* **84**, 062706 (2011).
- [23] Y. Suzuki and K. Varga, *Stochastic Variational Approach to Quantum-Mechanical Few-Body Problem* (Springer-Verlag, Berlin, 1998).
- [24] J. von Stecher, *J. Phys. B* **43**, 101002 (2010).
- [25] L. Platter, H.-W. Hammer, and U. Meißner, *Phys. Rev. A* **70**, 052101 (2004); H.-W. Hammer and L. Platter, *Eur. Phys. J. A* **32**, 113 (2007); J. von Stecher, J. P. D'Incao, and C. H. Greene, *Nature Phys.* **5**, 417 (2009); F. Ferlaino, S. Knoop, M. Berninger, W. Harm, J. P. D'Incao, H.-C. Nägerl, and R. Grimm, *Phys. Rev. B* **102**, 140401 (2009).
- [26] F. M. Penkov, *Phys. Rev. A* **60**, 3756 (1999); E. Nielsen, H. Suno, and B. D. Esry, *ibid.* **66**, 012705 (2002); F. Werner, *Europhys. Lett.* **86**, 66006 (2009).
- [27] T. Tscherble, S. T. Rittenhouse, and J. von Stecher (to be published).
- [28] W. Krauth, M. Caffarel, and J.-P. Bouchaud, *Phys. Rev. B* **45**, 3137 (1992).
- [29] D. S. Rokhsar and B. G. Kotliar, *Phys. Rev. B* **44**, 10328 (1991).
- [30] M. Foss-Feig and A. M. Rey, *Phys. Rev. A* **84**, 053619 (2011).
- [31] N. Gemelke, X. Zhang, C.-L. Hung, and C. Chin, *Nature (London)* **460**, 995 (2009).
- [32] F. Gerbier, *Phys. Rev. Lett.* **99**, 120405 (2007).