

# Phase diagram of one-dimensional hard-core bosons with three-body interactions

B. Capogrosso-Sansone,<sup>1</sup> S. Wessel,<sup>2</sup> H. P. Büchler,<sup>2</sup> P. Zoller,<sup>3,4</sup> and G. Pupillo<sup>3,4</sup>

<sup>1</sup>*Department of Physics, University of Massachusetts, Amherst, Massachusetts 01003, USA*

<sup>2</sup>*Institute for Theoretical Physics III, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany*

<sup>3</sup>*Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria*

<sup>4</sup>*Institute for Quantum Optics and Quantum Information, 6020 Innsbruck, Austria*

(Received 15 September 2008; published 9 January 2009)

We determine the phase diagram of a one-dimensional system of hard-core lattice bosons interacting via repulsive three-body interactions by analytic methods and extensive quantum Monte Carlo simulations. Such three-body interactions can be derived from a microscopic theory for polar molecules trapped in an optical lattice. Depending on the strength of the interactions and the particle density, we find superfluid and solid phases, the latter appearing at an unconventional filling of the lattice and displaying a coexistence of charge-density wave and bond orders.

DOI: [10.1103/PhysRevB.79.020503](https://doi.org/10.1103/PhysRevB.79.020503)

PACS number(s): 05.30.Jp, 03.75.Hh, 03.75.Lm, 75.40.Mg

## I. INTRODUCTION

Quantum many-body systems provide a wealth of fascinating phenomena in condensed-matter physics, including superfluidity in liquid helium, the fractional quantum Hall effect, as well as the exotic electronic states in the pseudogap regime of cuprate superconductors. While these quantum phases emerge from dominant two-body interactions, with higher-order many-body interaction terms providing only small corrections, an exciting recent avenue of research in atomic and molecular physics is to engineer systems where higher-order interactions dominate. In particular, it was recently shown that this goal can be achieved for three-body interactions using polar molecules.<sup>1</sup> In the present work, we study the most fundamental model Hamiltonian which displays three-body interactions in one dimension via quantum Monte Carlo (QMC) simulations.

One-dimensional bosonic systems in the strongly correlated regime have recently been realized with cold atomic gases: examples are the superfluid (SF) to Mott-insulator quantum phase transition for atoms trapped in optical lattices<sup>2,3</sup> and the crossover into the hard-core (Tonks-Girardeau) regime.<sup>4</sup> A characteristic feature of hard-core bosons in a lattice with additional off-site two-body interactions is the appearance of solid phases at half-filling  $n=1/2$  with either a charge-density wave (CDW) or a bond-ordered wave (BOW) phase.<sup>5,6</sup>

In contrast, here we study hard-core bosons with strong three-body interactions. While the microscopic realization of the model with polar molecules gives rise to next-nearest-neighbor (NNN) two-body and three-body interactions,<sup>1</sup> the dominant part of the Hamiltonian is

$$H = -J \sum_i [b_i^\dagger b_{i+1} + b_i b_{i+1}^\dagger] + W \sum_i n_{i-1} n_i n_{i+1}. \quad (1)$$

The first term describes the standard kinetic energy with hopping rate  $J$ , while the second term accounts for the three-body interaction with strength  $W$ ;  $n_i = b_i^\dagger b_i$  is the density operator with bosonic operators  $b_i$  and  $b_i^\dagger$  satisfying the hard-core constraint. A similar model has recently been studied in two dimensions.<sup>7</sup>

We derive the complete quantum phase diagram of Hamiltonian (1) by means of extensive quantum Monte Carlo simulations. We find the existence of both SF and solid phases (see Fig. 1). However, in contrast to systems with two-body interactions, we show that the solid phase appearing at the unconventional filling  $n=2/3$  exhibits both CDW and BOW orders. While Luttinger liquid (LL) theory predicts also instabilities toward a solid phase at  $n=1/2$  and  $n=1/3$ , we show here that the system remains superfluid even for strong three-body interactions  $W/J \gg 1$ . Solid phases at filling  $n=1/2$  are found by adding *weak two-body* nearest-neighbor (NN) and NNN corrections to Eq. (1),  $V_1 \sum_i n_i n_{i+1}$  and  $V_2 \sum_i n_i n_{i+2}$ , respectively, as naturally realized with polar molecules.<sup>1</sup>

## II. RESULTS

The ground-state phase diagram of the model in Eq. (1) is derived in the grand-canonical ensemble by varying the chemical potential  $\mu$  at different fixed values of  $W/J$ . We use two different QMC methods: (i) the stochastic series-expansion (SSE) algorithm with a generalized directed loop update<sup>8</sup> after a decoupling of the Hamiltonian in trimers for each three-body interaction term and (ii) a code based on the

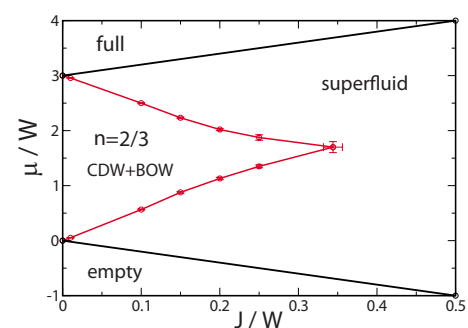


FIG. 1. (Color online) (QMC method: WA) Phase diagram of hard-core lattice bosons with dominant three-body interactions [Eq. (1)] in the grand-canonical ensemble,  $\mu/W$  vs  $J/W$ . The solid phase at filling  $n=2/3$  is characterized by a coexistence of CDW and BOW orders.

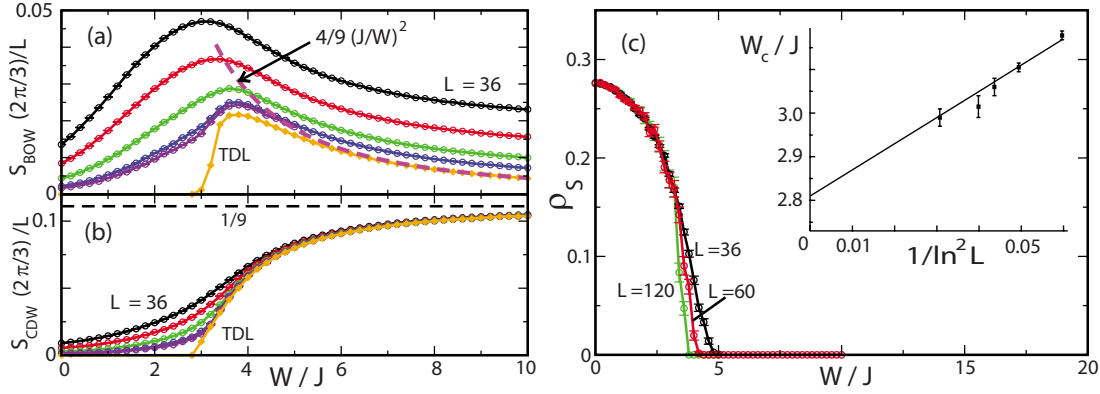


FIG. 2. (Color online) (QMC method: SSE) Lattice filling  $n=2/3$ . (a) Bond-order structure factor  $S_{\text{BOW}}(2\pi/3)/L$  vs  $W/J$ . Top to bottom: lattice sizes  $L=36, 60, 120, 240$ , and  $300$ ; the TDL is indicated. Dashed line: strong-coupling perturbative result  $4/9(J/W)^2$ . (b) Density structure factor  $S_{\text{CDW}}(2\pi/3)/L$  vs  $W/J$ . Top to bottom: lattice sizes  $L=36, 60, 120, 240$ , and  $300$ ; the TDL is indicated. Dashed line: strong-coupling result  $n^2/4=1/9$ . (c) Superfluid density  $\rho_s$  as a function of  $W/J$  for lattice sizes  $L=36, 60$ , and  $120$ . Inset:  $W_c/J$  as a function of  $1/\ln^2 L$  results from the WA. The line is a guide for the eyes.

Worm algorithm (WA) path-integral approach,<sup>9</sup> which allows efficient sampling of the many-body path winding numbers in imaginary time and space directions. Although the SSE method samples both BOW and CDW orders, its efficiency drops for very large values of  $W/J$ . The WA does not suffer from this issue and is especially useful in checking the limit  $W/J \gg 1$ . Results obtained with the two methods are found to be consistent (see below). The ground-state properties of the finite systems have been probed using temperatures  $T=0.6J/L$ , with  $L$  the number of lattice sites, which was found sufficiently low.

The phase diagram is determined by two phases (see Fig. 1): a superfluid LL phase with algebraic correlations, surrounding a solid phase at filling  $n=2/3$ , which appears for dominant three-body interactions  $W/J \gtrsim 3$ . The solid phase is incompressible, giving rise to the characteristic lobe structure in the  $\mu$ - $W$  phase diagram. This incompressible phase is characterized by the structure factors  $S_{\text{CDW}}$  for a charge-density wave and  $S_{\text{BOW}}$  for a bond-order wave at the wave vector  $k=2\pi/3$ ,

$$S_{\text{CDW}}(k) = \frac{1}{L} \sum_{j,l} \exp[ik(j-l)] \langle n_j n_l \rangle, \quad (2)$$

$$S_{\text{BOW}}(k) = \frac{1}{L} \sum_{j,l} \exp[ik(j-l)] \langle K_j K_l \rangle, \quad (3)$$

with the bond operators  $K_l = b_l^\dagger b_{l+1} + b_l b_{l+1}^\dagger$ .

The presence of CDW order can be easily understood in the limit  $J=0$ , where the ground state at filling  $n=2/3$  is threefold degenerate. In fact, up to lattice translations, each ground state takes the form  $|\Omega\rangle = \prod_k b_{3k}^\dagger b_{3k+2}^\dagger |0\rangle$  and exhibits CDW order with  $S_{\text{CDW}}(2\pi/3) = n^2 L/4$ . From the unconventional filling  $n=2/3$  of the solid phase, it follows that once hopping of particles is allowed the charge-density order implies small hopping correlations since the position of a particle in the solid breaks the symmetry of hopping to the left or hopping to the right. Using standard perturbation theory in the hopping term, we find that also a bond-order wave ap-

pears for finite hopping with  $S_{\text{BOW}}(2\pi/3) = n^2 L J^2 / W^2$ . Monte Carlo results directly confirm the coexistence of the two orders. Analogous to the case of the Hubbard model with on site two-body interactions, this incompressible phase at filling  $n=2/3$  can be reached by varying the density, which corresponds to a mean-field transition, or by keeping the density constant and by varying the strength of the interactions  $W/J$  (see Fig. 1). We found that the superfluid density vanishes at the boundaries, indicating that doping of the system happens simultaneously to the solid to SF transition. In the following we will be mainly interested in characterizing the constant-density transition at the tip of the lobe.

### A. Filling $n=2/3$

Our results for the order parameters  $S_{\text{BOW}}$  and  $S_{\text{CDW}}$  at fixed density  $n=2/3$  are shown in Fig. 2 for system sizes  $L=36, 60, 120, 240$ , and  $300$  (top to bottom), together with the extrapolated thermodynamic limit (TDL) behavior. The latter has been obtained based on an observed linear scaling of  $S_{\text{BOW}}$  and  $S_{\text{CDW}}$  in  $1/L$  within the solid phase and is found to be in perfect agreement with the strong-coupling results for the order parameters valid for  $W/J \gg 1$  (dashed lines). In the thermodynamic limit, the two order parameters are found to vanish simultaneously at a critical ratio  $W_c/J \approx 2.9$ , corresponding to the solid to liquid transition at the tip of the lobe.

A more refined determination of the transition point can be obtained using bosonization techniques. In the weakly interacting regime with  $W/J \ll 1$ , the system can be mapped onto the sine-Gordon model,<sup>1</sup>

$$H = \frac{\hbar v}{2} \int dx \left\{ \left[ K \Pi^2 + \frac{1}{K} (\partial_x \Phi)^2 \right] + \lambda \cos(\gamma \Phi) \right\}, \quad (4)$$

where  $\Phi$  denotes the charging field and  $\Pi$  the canonical conjugate operator, while  $K$  is the LL parameter and  $\gamma = \sqrt{36\pi}$  is the periodicity of the sine term. Consequently, the transition from the LL to the solid phase at the tip of the lobe in Fig. 1 appears at the critical value  $K_c = 2/9$  and it belongs to the Kosterlitz-Thouless (KT) universality class.<sup>11(b)</sup> For weak in-

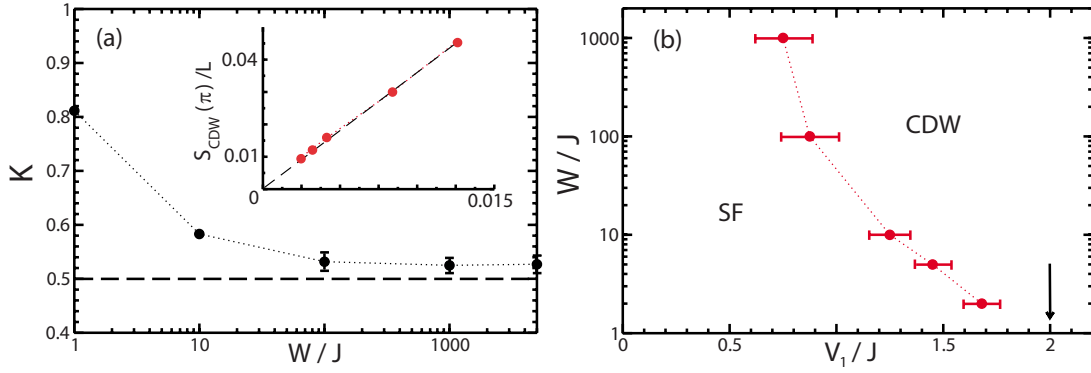


FIG. 3. (Color online) (QMC method: WA) Lattice filling  $n=1/2$ . (a) Luttinger liquid parameter  $K$  as a function of  $W/J$  with critical value  $K_c=0.5$  (dashed line) of the superfluid to solid transition. The inset shows the density structure factor  $S_{\text{CDW}}(\pi)/L$  as a function of the inverse system size  $1/L$  for  $W/J=1000$ . (b) Phase diagram in the presence of an additional nearest-neighbor interaction  $V_1$  in the plane  $W/J$  vs  $V_1/J$ . The arrow indicates the point of the superfluid to solid transition at  $W/J=0$ .

teractions  $W/J \ll 1$  the behavior of the Luttinger parameter is obtained directly from bosonization techniques as  $K=1 - (2\sqrt{3}/\pi)W/J$ ; however, this value is strongly renormalized close to the liquid to solid quantum phase transition. We compute the LL parameter numerically as  $K=\hbar\pi\sqrt{\rho_s\kappa}/m$  by QMC methods, with  $\rho_s$  and  $\kappa$  as the superfluid density and compressibility, respectively. The latter are calculated from the statistics of winding numbers  $\langle W_\alpha^2 \rangle$  in imaginary time and space directions. In particular, for a square system such that  $L_\tau \approx L_x = L$ , with  $L_\tau = \hbar v/T$  and  $v = \sqrt{\rho_s/\kappa m}$  the sound velocity,  $\rho_s = mL T \langle W_x^2 \rangle / \hbar^2$  (Ref. 10) and  $\kappa = \langle W_\tau^2 \rangle / LT$ , respectively, with  $m = \hbar^2/2J$ . We have performed simulations for  $L=60, 90, 120, 150$ , and  $300$ . In order to precisely locate the critical point we employ finite-size scaling arguments following from the KT renormalization-group flow.<sup>11</sup> Calling  $W_c(L)$  the value of  $W$  for which  $K(L)=K_c$ , the finite-size scaling of the transition point is  $W_c(L) - W_c \propto [\ln(L)]^{-2}$ , with  $W_c$  as the transition point in the thermodynamic limit. The inset of Fig. 2(c) shows the finite-size scaling of  $W_c(L)$ , which gives the transition point  $W_c/J = 2.80 \pm 0.15$ , in agreement with the discussion above.

### B. Filling $n=1/2$

In Ref. 1 it is argued that for lattice filling  $n=1/2$  a superfluid to solid transition should occur as a function of  $W/J$  at a critical LL parameter  $K_c=0.5$ . This instability is based on the observation that replacing the density operator by its fluctuations around the mean value  $n_i = n + \delta n_i$ , the three-body interaction gives rise to nearest-neighbor and next-nearest-neighbor interactions,

$$W \sum_i n_{i-1} n_i n_{i+1} \sim W n \sum_i [\delta n_{i-1} \delta n_{i+1} + 2 \delta n_{i-1} \delta n_i].$$

In analogy to systems with two-body interactions, one would expect a solid phase at half-filling  $n=1/2$ . However, we find that the competition between the nearest-neighbor interaction of strength  $2Wn$ , which drives an instability toward a CDW solid, and the next-nearest-neighbor interaction of strength  $Wn$ , which drives an instability toward a BOW solid, removes all instabilities altogether (see below). The

low-temperature phase is thus a superfluid, independent of the magnitude of  $W/J$ . This behavior is a special property of three-body interactions, and it is in stark contrast to the two-body case, where a transition into the solid phase has been always reported.<sup>5</sup> In Fig. 3(a) we show our results for  $K$  as a function of  $W/J$ , obtained using the procedure described above for system sizes  $L=80, 120, 160, 240$ , and  $320$ . For weak three-body interactions  $W/J \leq 1$ ,  $K$  tends to the hard-core value  $K=1$ . We find that for large interactions  $W/J \gg 1$  the LL parameter saturates at a value  $K=0.528 \pm 0.015 > K_c$  which is larger than the critical value  $K_c=0.5$ , and thus no superfluid to solid transition occurs at filling  $n=1/2$ . Consistently, the superfluid fraction does not show any appreciable system-size dependence (Fig. 4).

The inset of Fig. 3(a) shows the structure factor  $S_{\text{CDW}}(\pi)$  as a function of the inverse system size  $1/L$  for the case of  $W/J=1000$ . The structure factor extrapolates to a value consistent with zero in the thermodynamic limit, consistent with a superfluid in this limit of large three-body interactions. It remains an open question whether there is an analytical result predicting the value of the Luttinger parameter for infinite three-body interactions in analogy to hard-core bosons with  $K=1$ .

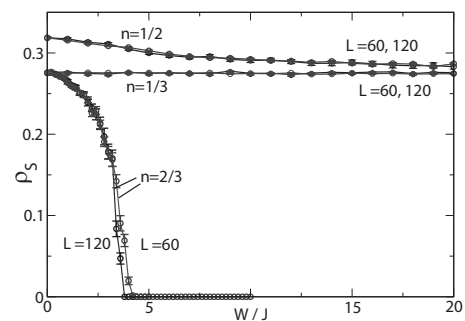


FIG. 4. (QMC method: SSE) Superfluid fraction  $\rho_s$  as a function of  $W/J$  for fillings  $n=1/3, 1/2$ , and  $2/3$ . Gray and black lines correspond to system sizes  $L=60$  and  $120$ , respectively. Due to particle-hole symmetry, the superfluid fractions for  $n=1/3$  and  $2/3$  are the same for  $W/J=0$ .

### C. Additional two-body interactions

We finally consider the effects of additional short-ranged two-body repulsions by adding to the model in Eq. (1) a term  $V_1 \sum_i n_i n_{i+1} + V_2 \sum_i n_i n_{i+2}$  with NN repulsion  $V_1$  and NNN repulsion  $V_2$ . Such terms are important as they constitute the leading correction to the short-range three-body repulsions considered thus far and can induce new instabilities of the LL. In fact, it is well known that a half-filled system of hard-core bosons with NN repulsions  $V_1$  undergoes a superfluid to CDW KT transition at  $V_1=2J$  to a twofold-degenerate state with ordering pattern  $\circ\circ\bullet$  ( $k=\pi$ ).<sup>12</sup>

In Fig. 3(b) we show how this transition is modified due to the presence of three-body interactions by presenting the low-energy phases as a function of  $W/J$  and  $V_1/J$ . We find that the presence of three-body interactions renormalizes considerably the SF/CDW transition by shifting it to lower values of  $V_1/J < 2$ . In particular, for  $W/J=1000$  we find  $V_1^c/J=0.75 \pm 0.15$ .

The presence of NNN interactions  $V_2 > 0$  can drive the system into a bond-ordered phase. In Ref. 5 it is shown that an ensemble of hard-core bosons with NNN interactions (at  $V_1=0$ ) enters a  $k=\pi$  bond-ordered phase for  $V_2/J=2.15 \pm 0.10$ . For even larger  $V_2/J > 2.66 \pm 0.10$ , a fourfold-degenerate  $k=\pi/2$  CDW phase with ordering pattern  $\circ\bullet\bullet\circ$  becomes stabilized. We find that the presence of three-body interactions significantly renormalizes these transition points. For example, at  $W/J=10$  the SF/BOW transition occurs for  $V_2/J=0.9 \pm 0.1$  and the BOW/CDW transition at  $V_2/J=2.1 \pm 0.1$ . Three-body interactions thus widen the extent of the BOW phase in this regime.

### D. Filling $n=1/3$

We find that at filling  $n=1/3$  the low-energy phase remains a superfluid independently of the strength of the three-

body interactions. Consistently, the superfluid fraction  $\rho_s$  in this case is found to be essentially independent of  $W/J$  in the range  $0 < W/J < 20$ , as seen in Fig. 4. We computed the value of the LL parameter for  $W/J=1000$  and found that  $K=0.89 \pm 0.01 > K_c=2/9$ , which confirms that three-body interactions alone do not induce a transition in this region. This finding contrasts the weak-coupling result<sup>1</sup> and exhibits the strong breaking of particle-hole symmetry by finite three-body interactions, as seen for  $W \neq 0$  from, e.g., comparing  $\rho_s$  for the two fillings  $n=1/3$  and  $n=2/3$  in Fig. 4. Adding a NN interaction also does not induce any transition at  $n=1/3$ . In fact, we find for  $W/J=1000$  and  $V_1/J=20$  that  $K=0.48 \pm 0.01 > K_c$ .

### III. CONCLUSIONS

We have determined the phase diagram of the fundamental model Hamiltonian for hard-core bosons with dominant short-range three-body interactions in one dimension. The latter can be realized with polar molecules cooled to the electronic and vibrational ground state, which is well in the reach of current experiments.<sup>13</sup> The one-dimensional nature of the problem opens fascinating prospects for studying the dynamics of systems with many-particle interactions by using powerful numerical techniques such as, e.g., adaptive time-dependent density matrix renormalization group (tDMRG).<sup>14</sup> Extensions to two dimensions<sup>7</sup> in various lattice geometries hold promises in the search for exotic phases, such as, e.g., topological phases and spin liquids.

### ACKNOWLEDGMENTS

We acknowledge discussions with N. V. Prokof'ev. This work was supported by the ESF with EuroQUAM, FWF, MURI, OLAQUI, and DARPA. Allocation of CPU time on NIC Jülich and HLRS Stuttgart is acknowledged.

<sup>1</sup>H. P. Büchler, A. Micheli, and P. Zoller, Nat. Phys. **3**, 726 (2007).

<sup>2</sup>T. Stöferle, Henning Moritz, Christian Schori, Michael Köhl, and Tilman Esslinger, Phys. Rev. Lett. **92**, 130403 (2004).

<sup>3</sup>C. D. Fertig, K. M. O'Hara, J. H. Huckans, S. L. Rolston, W. D. Phillips, and J. V. Porto, Phys. Rev. Lett. **94**, 120403 (2005).

<sup>4</sup>T. Kinoshita, T. R. Wenger, and D. S. Weiss, Science **305**, 1125 (2004); B. Paredes, A. Widera, V. Murg, O. Mandel, S. Fölling, I. Cirac, G. Shlyapnikov, T. Hänsch, and I. Bloch, Nature (London) **429**, 277 (2004).

<sup>5</sup>P. Schmitteckert and R. Werner, Phys. Rev. B **69**, 195115 (2004).

<sup>6</sup>T. D. Kühner and H. Monien, Phys. Rev. B **58**, R14741 (1998); R. D. Somma and A. A. Aligia, *ibid.* **64**, 024410 (2001).

<sup>7</sup>K. P. Schmidt, J. Dorier, and A. M. Läuchli, Phys. Rev. Lett. **101**, 150405 (2008).

<sup>8</sup>A. W. Sandvik, Phys. Rev. B **59**, R14157 (1999); O. F. Syljuåsen and A. W. Sandvik, Phys. Rev. E **66**, 046701 (2002).

<sup>9</sup>N. V. Prokof'ev, B. V. Svistunov, and I. S. Tupitsyn, Phys. Lett. A **238**, 253 (1998); JETP **87**, 310 (1998).

<sup>10</sup>E. L. Pollock and D. M. Ceperley, Phys. Rev. B **36**, 8343 (1987).

<sup>11</sup>(a) V. L. Berezinskii, Sov. Phys. JETP **34**, 610 (1972); (b) J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).

<sup>12</sup>M. Kohno and M. Takahashi, Phys. Rev. B **56**, 3212 (1997).

<sup>13</sup>S. Ospelkaus, A. Pe'er, K.-K. Ni, J. J. Zirbel, B. Neyenhuis, S. Kotochigova, P. S. Julienne, J. Ye, and D. S. Jin, Nat. Phys. **4**, 622 (2008); J. G. Danzl, E. Haller, M. Gustavsson, M. J. Mark, R. Hart, N. Bouloufa, O. Dulieu, H. Ritsch, and H.-C. Nägerl, Science **321**, 1062 (2008); J. Deiglmayr, A. Grochola, M. Repp, K. Mörtilbauer, C. Glück, J. Lange, O. Dulieu, R. Wester, and M. Weidemüller, Phys. Rev. Lett. **101**, 133004 (2008).

<sup>14</sup>G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003); S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); K. Mäsinger and U. Schollwöck, Phys. Rev. Lett. **81**, 445 (1998).