Quantum liquid of repulsively bound pairs of particles in a lattice

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Repulsively interacting particles in a periodic potential can form bound composite objects, whose dissociation is suppressed by a band gap. Nearly pure samples of such repulsively bound pairs of cold atoms—"dimers"—have recently been prepared by Winkler *et al.* [Nature (London) **441**, 853 (2006)]. We here derive an effective Hamiltonian for a lattice loaded with dimers only and discuss its implications for the many-body dynamics of the system. We find that the dimer-dimer interaction includes strong on-site repulsion and nearest-neighbor attraction which always dominates over the dimer kinetic energy at low temperatures. The dimers then form incompressible, minimal-surface "droplets" of a quantum lattice liquid. For low lattice filling, the effective Hamiltonian can be mapped onto the spin-1/2 *XXZ* model with fixed total magnetization which exhibits a first-order phase transition from the droplet to a gas phase. This opens the door to studying first-order phase transitions using highly controllable ultracold atoms.

I. INTRODUCTION

Many-body systems in spatially periodic potentials have been investigated since the early days of quantum theory [1]. Idealized descriptions such as the Heisenberg spin and Hubbard models have been used to examine basic issues in condensed matter physics. The Hubbard model has recently acquired direct experimental significance, however, describing cold atomic gases trapped in optical lattices [2]. The relevant parameters of these systems can be tuned to implement the Hubbard model with a remarkable accuracy. In particular, the transition from the superfluid to the Mott insulator phase [3] with a commensurate number of bosonic atoms per site has been demonstrated [4,5]. More recently, Winkler *et al.* [6] have observed another lattice effect: binding of *repulsively* interacting bosons into close pairs which are dynamically stable in the absence of dissipation. Repulsively bound composite objects are a general phenomenon, appearing in various periodic systems possessing a band gap at the relevant "dissociation" energy. Electrons have been shown to pair, via Coulomb repulsion, in arrays of tunnel-coupled quantum dots [7]. Analogous effects have been predicted for strongly interacting mixtures of bosonic and fermionic atoms in an optical lattice [8], or photons forming gap solitons in nonlinear photonic band gap structures [9].

Here we study a lattice loaded with even numbers of bosonic atoms at each site, in the experimentally relevant regime [6] where the on-site repulsion between atoms exceeds the intersite tunneling rate. We derive an effective Hamiltonian for repulsively bound atom pairs ("dimers"), which describes the many-body dynamics of the pairs, viewed as single composite objects. A special property of the system, not shared by less exotic systems, is the effective occupation-dependent tunneling and nearest-neighbor interactions of the dimers mediated by the single-atom tunneling via nonresonant virtual states. We find that the attractive interaction between the dimers always exceeds their kinetic energy which, combined with the still stronger on-site repulsion that the dimers inherit from the repulsion among their

constituent atoms, leads to clustering of the dimers into "droplets" with minimum surface area and uniform density. When the system is initially prepared with at most one dimer per site [6], the effective Hamiltonian can be mapped onto the spin-$\frac{1}{2}$ *XXZ* model [10] with fixed magnetization, which is known to exhibit a first-order phase transition from a droplet to a "gas" phase at a critical temperature [11].

II. REPULSIVELY BOUND DIMER WITHIN THE BOSE-HUBBARD MODEL

The dynamics of cold bosonic particles occupying the lowest Bloch band of a tight-binding periodic potential is governed by the Bose-Hubbard Hamiltonian ($\hbar = 1$)

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

where $b_j^\dagger$ (b_j) is the creation (annihilation) operator for a boson at site j with energy ε_j, U is the on-site interaction (repulsion for $U > 0$), $\hat{n}_j = b_j^\dagger b_j$ is the number operator for site j, and J is the tunneling rate between adjacent sites $\langle j,i \rangle$. A natural basis for the Hamiltonian (1) is that of the eigenstates $|n_j\rangle \equiv (1/\sqrt{n!})(b_j^\dagger)^n|0\rangle$ of the number operator $\hat{n}_j$ whose eigenvalues $n = 0,1,2,\ldots$ denote the number of particles at site j, and $|0\rangle \equiv |\{0_j\}\rangle$ is the vacuum state. For a single particle in a uniform ($\varepsilon_j = \varepsilon$ for all j) periodic potential, the on-site interaction plays no role, and resonant tunneling leads to a Bloch band of width $4dJ$ centered around ε, where d is the system dimension.

Considering next two particles in a periodic potential, according to Eq. (1), the state $|2_j\rangle$ with two particles localized at the same site has an energy offset U from the state $|1_j\rangle|1_i\rangle$ with $i \neq j$. The transition between states $|1_j\rangle|1_i\rangle$ and $|2_j\rangle$ is therefore nonresonant and is suppressed when $U \gg J$. If initially the particles occupy different sites, each particle can tunnel freely from site to site, until it encounters the other particle at a neighboring site. At this point the two particles undergo elastic scattering and separate again, since the maxi-

mal kinetic energy $4dJ$ of the two particles is below the potential barrier U associated with two particles occupying the same site. Note that, in second order in the small parameter J/U, an adiabatic elimination of the nonresonant states $|2_j\rangle$ and $|2_i\rangle$ yields an effective energy shift of state $|1_j\rangle|1_i\rangle$ with two particles at the adjacent sites $\langle j, i \rangle$, given by $-4J^2/U$. This effective attraction between a pair of particles at the neighboring sites is, however, small compared to the single-particle tunneling rate J, and therefore cannot bind the particles together. Conversely, if the system is initially prepared in state $|2_j\rangle$, then in order for the two particles to separate ($|2_j\rangle \rightarrow |1_j\rangle|1_i\rangle$) via the last term of Eq. (1), energy of the order of U would have to be discarded. In the absence of dissipation, this is not possible, so the two particles are repulsively bound as a dimer [6]. Using the perturbative analysis outlined in Appendix A, it is easy to show that the localization (or "bond") length of the dimer is $\zeta = [2 \ln(U/dJ)]^{-1}$, so that $\zeta < 1$ for $U/J > d\sqrt{e}$. Hence, the dimer constituents are strongly colocalized for $U/J \gg 1$, which will be assumed from now on.

An important aspect of the problem is the dimer mobility. Although the first-order transition $|2_j\rangle \rightarrow |1_j\rangle|1_i\rangle$ (with j and i denoting adjacent sites) effected by the last term of Eq. (1) is nonresonant, in the second order in J, the transition $|2_j\rangle \rightarrow |2_i\rangle$ via the virtual intermediate state $|1_j\rangle|1_i\rangle$ is resonant. An adiabatic elimination [13] of the intermediate state $|1_j\rangle|1_i\rangle$ then yields an effective tunneling rate for a dimer as a whole, given by $J^{(2)} \equiv 2J^2/U \ll J$. Note also that the adiabatic elimination of $|1_j\rangle|1_i\rangle$ results in an energy shift of the dimer states $|2_j\rangle$ equal to $J^{(2)}$, which constitutes a correction to the dimer energy $2\varepsilon + U$. In analogy with the single-particle case, the effective tunneling with the rate $J^{(2)}$ implies a narrow Bloch band for single dimers, of width $4dJ^{(2)}$ centered around $2\varepsilon + U + J^{(2)}$.

III. EFFECTIVE HAMILTONIAN FOR A SYSTEM OF DIMERS

So far, we have discussed the properties of a single repulsively bound dimer in a periodic potential. Our aim next will be to describe the dynamics of a system of dimers. We know no useful exact analytic treatments, but for $J \ll U$ the perturbation approach outlined in Appendix A can be extended to this problem straightforwardly. Expressing the particle number as $n = 2m$, where $m = 0, 1, 2 \ldots$ represents the number of dimers at a given site, we denote the state containing m dimers at site j as $|m_j^D\rangle$. It is convenient to define the operators $c_j = [1/\sqrt{2(\hat{n}_j + 1)}]b_j^2$, and $c_j^\dagger = (b_j^\dagger)^2[1/\sqrt{2(\hat{n}_j + 1)}]$, which annihilate and create a dimer at site j. Within the subspace of states in which all occupation numbers are even, these operators behave exactly as canonical creation and annihilation operators, possessing the standard bosonic commutation relations $[c_j, c_i^\dagger] = \delta_{ji}$ and $[c_j, c_i] = [c_j^\dagger, c_i^\dagger] = 0$. The dimer number operator at site j is then given by $\hat{m}_j = c_j^\dagger c_j = \hat{n}_j/2$. It is easy to verify by induction that $|m_j^D\rangle \equiv (1/\sqrt{m!})(c_j^\dagger)^m|0\rangle$.

We can now derive an effective Hamiltonian H_{eff} for a periodic potential loaded with dimers only [6]. To zeroth order in the tunneling interaction J, only the first two terms
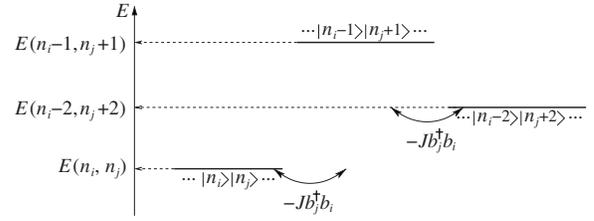
FIG. 1. Energy level diagram and tunnel couplings employed in the adiabatic elimination of nonresonant states with odd occupation numbers. $\cdots |n_i\rangle|n_j\rangle \cdots$ denotes a state with $n_i = 2m_i$ bosons at site i and $n_j = 2m_j$ bosons at site $j = i + 1$, etc., while the energy is $E(n_i, n_j) = (U/2)[n_i(n_i - 1) + n_j(n_j - 1)] + C$, where C contains the energy of all the other sites.

of Eq. (1) survive. In terms of the dimer operators we have defined, they are given, respectively, by $2\varepsilon \Sigma_j \hat{m}_j$ and $U \Sigma_j \hat{m}_j (2\hat{m}_j - 1)$. To first order in J, under the condition of the strong on-site repulsion $U \gg J$, all the states containing odd numbers of particles per site will be nonresonant, and can be eliminated adiabatically [13]. The energy diagram of the eigenstates is shown in Fig. 1, using which we obtain in the second order in J/U [14]

$$H_{\text{eff}} = 2\varepsilon \sum_j \hat{m}_j + U \sum_j \hat{m}_j(2\hat{m}_j - 1)$$
$$+ J^{(2)} \sum_{\langle j,i \rangle} c_j^\dagger \hat{T}(\hat{m}_j, \hat{m}_i) c_i + J^{(2)} \sum_{\langle j,i \rangle} \hat{S}(\hat{m}_j, \hat{m}_i), \quad (2)$$

where $J^{(2)} \equiv 2J^2/U$, and $\hat{T}$ and $\hat{S}$ are defined as

$$\hat{T}(\hat{m}_j, \hat{m}_i) = \delta_{\hat{m}_i \hat{m}_j} \sqrt{(2\hat{m}_j + 1)(2\hat{m}_i + 1)}, \quad (3a)$$

$$\hat{S}(\hat{m}_j, \hat{m}_i) = \frac{\hat{m}_i(2\hat{m}_j + 1)}{2\hat{m}_i - (2\hat{m}_j + 1)}. \quad (3b)$$

The third term on the right-hand side of Eq. (2) describes dimer tunneling between adjacent sites. This tunnel interaction is resonant only between states of the form $|m_j^D\rangle|(m+1)_i^D\rangle$ and $|(m+1)_j^D\rangle|m_i^D\rangle$, for which the occupation numbers of the adjacent sites differ by 1; the corresponding matrix element is equal to $J^{(2)}(m+1)(2m+1)$. The last term of Eq. (2), containing the energy shift function $\hat{S}$, is responsible for the nearest-neighbor interaction, which, depending on the values of m_j and m_i, can be positive or negative. Adding the two interaction terms between adjacent sites i and j, we arrive at

$$\hat{S}(\hat{m}_j, \hat{m}_i) + \hat{S}(\hat{m}_i, \hat{m}_j) = \frac{2\hat{m}_j^2 + 2\hat{m}_i^2 + \hat{m}_j + \hat{m}_i}{4(\hat{m}_j - \hat{m}_i)^2 - 1}. \quad (4)$$

Thus, when $m_j = m_i$ the interaction between neighboring sites is attractive; otherwise it is repulsive. These effects can be understood as level shifts of the dimer states, due to "level repulsion" from virtual states having odd occupation numbers. The Hamiltonian (2) describes the effective dynamics of dimers in a one- (1D), two- (2D), or three-dimensional (3D) periodic potential, in the strong-coupling regime. Its key features are occupation-dependent tunneling and nearest-

neighbor interactions, as well as strong on-site repulsion via the term proportional to U.

It is instructive to consider a 1D configuration

$$\cdots |m^D_{j-2}\rangle |m^D_{j-1}\rangle |(m+1)^D_j\rangle |(m+1)^D_{j+1}\rangle \cdots ,$$

which involves the occupation number m of a pair of adjacent sites $j-2$ and $j-1$, and the occupation number $m+1$ of sites j and $j+1$. According to Eq. (4), there are attractive interactions between sites $j-2$ and $j-1$, and between sites j and $j+1$, while sites $j-1$ and j, having different occupation numbers, interact repulsively. Then the total potential energy is the sum of the three terms given by $s=-J^{(2)}\frac{5}{3}(4m^2+6m+3)$. Due to the very large on-site repulsion proportional to $U \gg J^{(2)}$, the only (near-)resonant tunneling interaction of the above state is with the state

$$\cdots |m^D_{j-2}\rangle |(m+1)^D_{j-1}\rangle |m^D_j\rangle |(m+1)^D_{j+1}\rangle \cdots ,$$

having potential energy $s'=J^{(2)}(4m^2+6m+3)$. The corresponding tunneling matrix element $t=J^{(2)}(m+1)(2m+1)$. Thus, the ratio of the tunneling (kinetic) energy to the change in the potential energy between the above two states is given by

$$\frac{t}{s'-s} = \frac{3(m+1)(2m+1)}{8(4m^2+6m+3)}. \tag{5}$$

This ratio is always smaller than 1, its minimal value being $1/8$ for $m=0$, and it quickly approaches a constant $3/16$ for $m>1$.

The tunneling $\hat{T}$ and the nearest-neighbor $\hat{S}$ interactions are responsible for competing processes: While tunneling favors dispersed dimer wave functions with long-range coherence, the nearest-neighbor attraction tends to balance the population of neighboring sites and to minimize the surface area between regions of different occupation numbers. Since the interaction term is always larger than the competing tunneling term, the ground state will be dominated by attractively bound clusters of uniform occupation number and minimal surface area, thus representing incompressible droplets of a quantum lattice liquid.

IV. EFFECTIVE HAMILTONIAN FOR $m \leq 1$

Let us now consider the important special case of a system containing at most one dimer per site ($m=0$ or 1 for all j). We thus assume that the periodic potential can be loaded initially only with zero or two particles per site, at effectively infinite U/J, which is then adiabatically lowered to a large but finite value, as implemented in the optical lattice experiment of Winkler *et al.* [6]. Just as dimers are energetically forbidden to dissociate in the absence of dissipation, the single-site dimer occupation numbers will never exceed unity, for this would require a large energy input of the order of $5U$. Under these conditions, the effective Hamiltonian (1) can be recast simply as

$$H^{(0,1)}_{\text{eff}} = (2\varepsilon + U + J^{(2)})\sum_j \hat{m}_j + J^{(2)}\sum_{\langle j,i \rangle} c^\dagger_j c_i - 4J^{(2)}\sum_{\langle j,i \rangle} \hat{m}_j \hat{m}_i, \tag{6}$$

where the only allowed values of m are 0 or 1. Thus, in addition to the tunneling interaction with negative effective mass, there is a stronger attractive interaction between dimers localized at neighboring sites, which can bind them together as discussed in Appendix B. Note that (6) has the form of an extended Hubbard model, like that which describes electrons in a crystal lattice or quantum dot array [7]. There, however, the nearest-neighbor interaction is repulsive, while in our case it is attractive. We also note that related effects have been predicted for strongly interacting mixtures of bosonic and fermionic atoms in an optical lattice [8], wherein the fermions tend to pair with one or more bosons, forming composite fermions with nearest-neighbor interaction.

To verify the validity of our perturbative approach in the limit of $J/U \ll 1$, we have numerically solved the Schrödinger equation for the cases of one and two dimers in a 1D lattice of 20 sites, using the Bose-Hubbard Hamiltonian (1), and the effective Hamiltonian (2) [or (6)]. As shown in Fig. 2, the dynamics of the system obtained from the exact and effective Hamiltonians is very similar; the difference between the exact and effective models decreases for smaller values of J/U, as expected. In the inset of Fig. 2(a) we plot the projection of the system wave function $|\Psi(t)\rangle$ onto the states $|2_j\rangle$ with two particles per site. As seen, $\Sigma_j |\langle 2_j | \Psi \rangle|^2 \simeq 1$ at all times, attesting to the fact that the two particles forming a dimer are strongly bound to each other, even though the center-of-mass wave function of the dimer disperses with time due to the tunneling $J^{(2)}$. Figures 2(c) and 2(d) reveal the greatly reduced dispersion for a pair of neighboring dimers attractively bound to each other (see Appendix B): the two-dimer pair collectively tunnels resonantly only at fourth order in the fundamental J (second order in $J^{(2)}$).

The above reasoning can be extended to the case of more dimers. Since each dimer is attracted to its immediate neighbor, for a given number of dimers, the configuration that minimizes the energy of the system would correspond to clustering of the dimers together in such a way as to maximize the number of nearest-neighbor (attractive) interactions. Thus, in 1D all the dimers would stick together in a line without voids, while for a 2D or 3D square lattice, the dimers would tend to arrange themselves in a square (2D) or a cube (3D), as shown in Fig. 3. (Because of the discretized perimeter metric in the lattice, minimal surfaces of these droplets are rectangular rather than round, however large.)

V. PHASE DIAGRAM OF THE GRAND CANONICAL ENSEMBLE

In order to understand the ground-state properties of the effective Hamiltonian (2), we consider the grand canonical ensemble described by the operator

$$K = H_{\text{eff}} - \mu \sum_j \hat{m}_j, \tag{7}$$

where μ is the chemical potential assumed uniform for all sites. The corresponding phase diagram, calculated numeri-
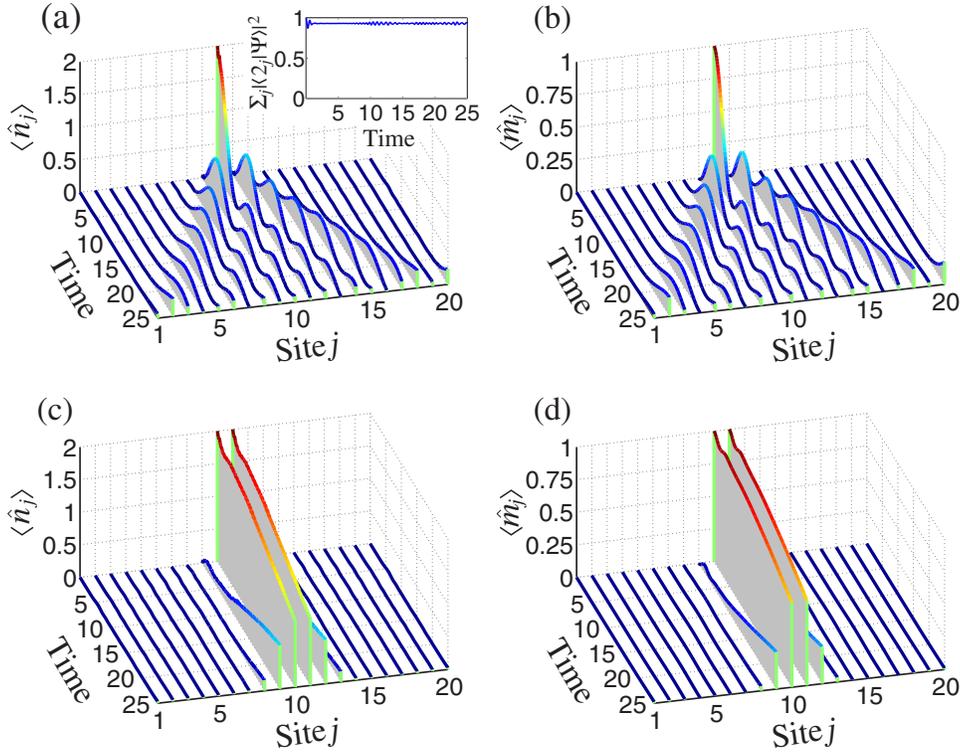
FIG. 2. (Color online) Dynamics of one dimer (a) and (b) and two dimers (c) and (d), in a 1D lattice of 20 sites, for $J/U=0.1$. (a) and (c) are numerical solutions of the Schrödinger equation with the Bose-Hubbard Hamiltonian (1), while (b) and (d) are obtained with the effective Hamiltonian (2) [or (6)]. Inset in (a) shows the time evolution of $\Sigma_j|\langle 2_j|\Psi\rangle|^2$, where $|\Psi(t)\rangle$ is the system wave function. Time is in units of J^{-1}.

cally for a small 1D lattice at zero temperature, is shown in Fig. 4. Since the tunneling interaction is always smaller than the attractive interaction between neighboring sites with equal occupation numbers, we observe only incompressible phases, with uniform, commensurate filling. All systems with incommensurate dimer filling lie on the border lines between the incompressible phases, which verifies the qualitative discussion above. When adding a dimer to the system, it is energetically favorable for this dimer to be bound to an already existing cluster or droplet rather than to move freely.

This picture changes, however, when a finite temperature T is considered. If T is sufficiently large the minimum free energy may be attained when the dimers move freely rather than being bound to a cluster. We thus expect the system to show a first-order phase transition from a quantum-droplet phase to a gas phase at some critical temperature T_c.

VI. DROPLET-GAS TRANSITION

The system described by the effective Hamiltonian $H_{\text{eff}}^{(0,1)}$ is equivalent to the well-known spin-$\frac{1}{2}$ *XXZ* model in a magnetic field [10,11]. Indeed, with the mapping $|0_j\rangle \rightarrow |\downarrow_j\rangle$ and $|1_j\rangle \rightarrow |\uparrow_j\rangle$ and simple algebraic manipulations, which essen-
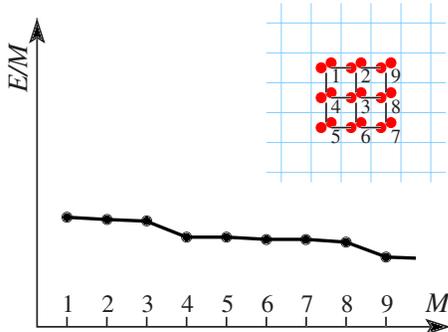
FIG. 3. (Color online) Energy per dimer E/M versus the number of dimers M forming a cluster in a 2D square lattice. As seen, E/M abruptly drops once a square droplet with the dimension $\sqrt{M} \times \sqrt{M}$ is formed, since the addition of the last dimer results in the formation of two "bonds."
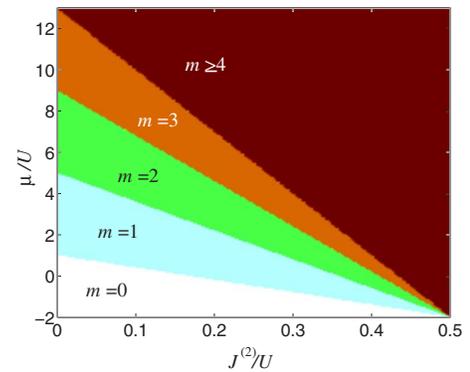
FIG. 4. (Color online) Phase diagram of the grand canonical ensemble obtained from exact diagonalization of Eq. (7). The Hilbert space is restricted by five sites (periodic boundary conditions), with each site occupation number in the range of $0 \le m \le 4$. The areas of integer filling are tightly adjoined to each other, with no significant extent of fractional filling phase.
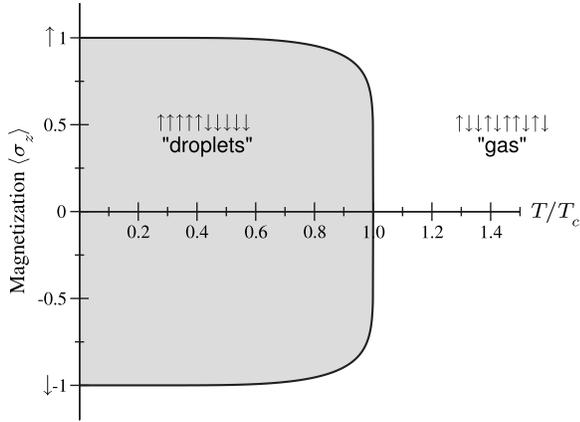
FIG. 5. Temperature phase diagram of the 2D Ising model. In the shaded area, the ferromagnetic spin domains are formed. As temperature is increased, for $\langle \sigma^z \rangle \neq 0$, the system undergoes a first-order phase transition to the gas phase, while at $\langle \sigma^z \rangle = 0$ it is a second-order phase transition. See text for more details.

tially amount to the Wigner-Jordan transformation, Eq. (6) can be cast as

$$H_{\text{spin}} = C - 2h_z \sum_j \sigma_j^z + \frac{J^{(2)}}{4} \sum_{\langle j,i \rangle} (\sigma_j^x \sigma_i^x + \sigma_j^y \sigma_i^y) - J^{(2)} \sum_{\langle j,i \rangle} \sigma_j^z \sigma_i^z,$$

(8)

where C is an immaterial constant, $h_z = 2dJ^{(2)} - \frac{1}{4}(2\varepsilon + U + J^{(2)})$ is an effective magnetic field, and σ_j^x, σ_j^y, and σ_j^z are the Pauli spin matrices. Note that, unlike the usual situation in spin systems, here the averaged "magnetization" of the system, $\langle \sigma^z \rangle$, is fixed by the condition $\langle m \rangle = (1 + \langle \sigma^z \rangle)/2$, where $\langle m \rangle$ is the dimer filling factor. In this description, we have a ferromagnetic spin coupling described by the last term of Eq. (8), which dominates over the spin-exchange interaction. At low temperatures ($k_B T < J^{(2)}$), the "spins" therefore form a ferromagnetic domain with the spins pointing up, surrounded by the remaining spins pointing down. At a certain critical temperature T_c, the spin domains disappear and a random distribution of the $|\uparrow_j\rangle$ and $|\downarrow_j\rangle$ states emerges. In order to estimate T_c, we note that in the above spin Hamiltonian the ZZ coupling is significantly larger than the XX and YY couplings, which, to a reasonable approximation, can be neglected. Equation (8) then reduces to the Ising Hamiltonian [15], whose analytic properties in 2D are well known. In Fig. 5 we show the finite-temperature phase diagram of the 2D Ising model. The shaded ferromagnetic spin domains at low temperatures correspond to the droplets of our model. The boundary of that region $\langle \sigma^z \rangle_c(T)$ is defined through

$$\langle \sigma^z \rangle_c(T) = \left[1 - \sinh^{-4} \left(\frac{2J^{(2)}}{k_B T} \right) \right]^{1/8}.$$

As the temperature is increased, for $\langle \sigma^z \rangle \neq 0$ the system undergoes a first-order phase transition from the droplet to the gas phase. For $\langle \sigma^z \rangle = 0$, the transition is a monotonic, second-order phase transition, for which the critical temperature

T_c corresponds to $\langle \sigma^z \rangle_c(T_c) = 0$, which yields $k_B T_c / J^{(2)} = 2/\text{arcsinh}(1) = 2.2692$.

VII. CONCLUSIONS AND CLOSING REMARKS

Before closing, let us briefly consider several important experimental issues. As we have stated in the beginning of this paper, the most relevant experimental situation for the present study is realized by cold bosonic atoms loaded into an optical lattice [6]. Initially, pairs of atoms (^{87}Rb) are adiabatically converted with near unit efficiency into chemically bound molecules (Rb$_2$) using a magnetic field sweep across a Feshbach resonance. This step is then followed by removing all chemically unbound atoms with combined radio-frequency and optical purification pulses. Finally, the dimer molecules are adiabatically converted back into pairs of atoms localized at the same site, with no significant admixture of unpaired atoms. In the case of strong on-site repulsion $U \gg J$, these pairs of atoms form the dimers studied in this paper. When the lattice sites are occupied by more than one dimer, the three- and four-body collisions will presumably be the dominant loss mechanism for the atoms. In a recent study, Campbell *et al.* [16] have experimentally realized a Mott insulator phase of cold ^{87}Rb atoms with per site particle numbers of $n = 1, 2, 3, 4, 5$ in successive spatial shells, and determined the lifetime of each shell. The observation for $n = 2$ was around 100 s, and for $n \geq 3$ around 0.5 s. On the other hand, the rate of dimer tunneling $J^{(2)}$ estimated from [6] is about $10-20$ s^{-1}, which is thus three orders of magnitude larger than the loss rate for $n = 2$ (i.e., $m = 1$), and an order of magnitude larger than the loss rate for $n = 4$ (i.e., $m = 2$).

In the experiment of Winkler *et al.* [6], in order to determine the fraction of remaining dimers for various experimental conditions and hold times, the authors repeat the above sequence (i.e., conversion of atom pairs into molecules, purification, and reverse conversion) and then use the conventional absorption imaging. With minor modification, this method can be employed to experimentally verify the formation of clusters of dimers. Recall that dimers forming a cluster become immobile, while individual unbound dimers are mobile, moving around the lattice with the tunneling rate $J^{(2)}$. Let us assume that at the boundaries of the lattice of linear dimension l there exists some dimer loss mechanism (see below). Then, if the dimers are not bound to each other, after a sufficient time of the order of $t_{\text{escape}} \sim l/J^{(2)}$, they will escape from the lattice, while immobile dimers bound in a cluster will remain in the lattice, which can be verified by the same absorption imaging. The loss mechanism at the boundaries of the lattice can be an atom evaporation by focused laser beams. Alternatively, if the lattice potential is created by a strongly focused (blue-detuned) laser field, then away from the central region, as the intensity of the field falls off, the tunneling barriers become lower. As a result, the dimer mobility increases, and eventually even individual atoms can move practically freely, quickly escaping the lattice.

Let us finally note that in the above discussion of the properties of repulsively bound pairs of particles in a periodic potential, we have neglected the effects of energy dissi-

pation in the system. Assuming small temperature and the dimer filling factor $\langle m \rangle \leqslant 1/2$ (average particle filling factor $\langle n \rangle \leqslant 1$), it is obvious that in the presence of energy relaxation with a characteristic rate γ (such as from spontaneous emission of phonons in a solid, or inelastic collisions with a cold background gas for atoms in an optical lattice), the lifetime of repulsively bound pairs will be limited by γ^{-1}. But for an initial random distribution of dimers in the lattice, dissipation on shorter time scales than γ^{-1} will drive formation of multidimer clusters, to minimize the energy of the dimer system. Furthermore, once a cluster is formed, dimer dissociation becomes a surface process only, because dissociation of a dimer inside the cluster would mean forming a "trimer" at an adjacent site, which requires energy input U, instead of energy release. Note also that the collision of a single unpaired particle with a dimer involves resonant single-particle exchange [14]. The admixture of single particles thus brings a complicated interplay between dimer dissociation and bound dimer collisions with single particles. Detailed understanding of fluctuations and dissipation in the liquidlike phase of clustered dimers will require further investigation, bringing the physics of first-order phase transitions into the arena of ultracold atoms.

ACKNOWLEDGMENTS

APPENDIX A: PERTURBATIVE DERIVATION OF A DIMER WAVE FUNCTION

The exact wave function and dispersion relation for single dimers can be obtained analytically in 1D [6,12]. As a tutorial for our derivation of the effective many-dimer Hamiltonian, we analyze the single dimer perturbatively for small J/U [3]. Given a dimer centered at site j, in 1D its "internal" state $|D_j\rangle$ is

$$|D_j\rangle = A_{j,0}|2_j\rangle + \sum_r (A_{j,r}|1_j\rangle|1_{j+r}\rangle + A_{j,-r}|1_{j-r}\rangle|1_j\rangle),$$
(A1)

where $r = 1, 2, \ldots$ is the distance in sites one of the constituent particles of the dimer has tunneled away from the other. In zeroth order in J, we have $A_{j,0} = 1$ and all $A_{j,\pm r} = 0$. At successively higher orders in J/U it is easy to see that $A_{j,\pm r} \simeq \sqrt{2}(-J/U)^r A_{j,0}$. The corresponding probability of finding the dimer constituents separated by r sites is $P_{j,r} = |A_{j,r}|^2 + |A_{j,-r}|^2 = 4P_{j,0}(J^2/U^2)^r$, while $P_{j,0} = |A_{j,0}|^2$. For $|J/U| \ll 1$, the normalization condition $\Sigma P_{j,r} = 1$ then yields

$$A_{j,0} \simeq \sqrt{\frac{U^2 - J^2}{U^2 + 3J^2}}, \quad A_{j,\pm r} \simeq (-1)^r \sqrt{2} A_{j,0}\left(\frac{J}{U}\right)^r. \quad \text{(A2)}$$

Note the alternating sign of the amplitudes $A_{j,\pm r}$ between the sites r. Expressing the tunneling probabilities $P_{j,r}$ as

$$P_{j,r} = 4P_{j,0} \exp\left[\ln\left(\frac{J^2}{U^2}\right)^r\right] = 4P_{j,0}e^{-r/\zeta}, \quad \text{(A3)}$$

we find the localization (or bond) length of the dimer to be $\zeta = [2\ln(U/J)]^{-1}$, so that $\zeta < 1$ for $U/J > \sqrt{e}$. These results agree with the exact expressions [6,12] in the limit $J \ll U$, and they can be extended to higher dimensions, which are less tractable by exact methods. Thus, for example, in 2D we obtain

$$A_{j,0} \simeq \sqrt{\frac{U^2 - 3J^2}{U^2 + 5J^2}}, \quad \text{(A4)}$$

$$P_{j,r} \simeq 8P_{j,0}\left(\frac{\Gamma\left(r + \frac{1}{2}\right)}{\sqrt{\pi}\Gamma(r+1)}4^r - 1\right)\left(\frac{J^2}{U^2}\right)^r$$

$$< 8P_{j,0} \exp\left[\ln\left(\frac{4J^2}{U^2}\right)^r\right] = 8P_{j,0}e^{-r/\zeta}, \quad \text{(A5)}$$

where the localization length is $\zeta = [2\ln(U/2J)]^{-1}$.

APPENDIX B: PERTURBATIVE DERIVATION OF TWO-DIMER WAVE FUNCTION

Consider a 1D configuration with two dimers occupying adjacent sites $\langle j, i \rangle$. Their potential energy is lower by the amount $8J^{(2)}$ than that of two dimers separated by one or more lattice sites [see Eq. (6)]. In analogy with the case of two particles forming a dimer, we can calculate the wave function $|Q_{ji}\rangle$ of the attractively bound dimer pair perturbatively in the effective tunneling $J^{(2)}$. To that end, we expand the wave function $|Q_{ji}\rangle$ as

$$|Q_{ji}\rangle = B_{ji,0}|1_j^D\rangle|1_i^D\rangle + \sum_r (B_{ji,r}|1_j^D\rangle|1_{i+r}^D\rangle + B_{ji,-r}|1_{j-r}^D\rangle|1_i^D\rangle),$$
(B1)

where $r = 1, 2, \ldots$ is the number of sites separating the dimers. We then obtain $B_{ji,\pm r} \simeq (-1/8)^r B_{ji,0}$, which, upon requiring the normalization $\Sigma P_{ji,r} = 1$, where $P_{ji,r} = |B_{ji,r}|^2 + |B_{ji,-r}|^2$ yields

$$B_{ji,r} \simeq \sqrt{\frac{63}{65}}\left(-\frac{1}{8}\right)^r. \quad \text{(B2)}$$

We therefore have $P_{ji,r} \simeq 2e^{-r/\xi}$ with the localization length $\xi = (\ln 64)^{-1} \simeq 0.24$. Hence, two dimers localized at adjacent lattice sites are closely bound to each other. It can be shown that this conclusion also holds in 2D and 3D.

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[14] Note that states of the form $|n_j\rangle|(n\pm1)_i\rangle$ and $|(n\pm1)_j\rangle|n_i\rangle$ (with $\langle j,i\rangle$) are resonantly coupled to each other via single-particle tunneling. But by assuming that only even numbers of particles per site are present initially in the system, we have explicitly excluded such events.

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