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Phillips, L. G.; De Chiara, G.; Ohberg, Patrik; Valiente, M.

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Low-energy behavior of strongly interacting bosons on a flat-band lattice above the critical filling factor

L. G. Phillips,[1] G. De Chiara,[2] P. Öhberg,[1] and M. Valiente[1]

[1]*SUPA, Institute of Photonics and Quantum Sciences, Heriot-Watt University, Edinburgh EH14 4AS, United Kingdom*

[2]*Centre for Theoretical Atomic, Molecular and Optical Physics, School of Mathematics and Physics, Queen's University, Belfast BT7 1NN, United Kingdom*

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Bosons interacting repulsively on a lattice with a flat lowest band energy dispersion may, at sufficiently small filling factors, enter into a Wigner-crystal-like phase. This phase is a consequence of the dispersionless nature of the system, which in turn implies the occurrence of single-particle localized eigenstates. We investigate one of these systems—the sawtooth lattice—filled with strongly repulsive bosons at filling factors infinitesimally above the critical point where the crystal phase is no longer the ground state. We find, in the hard-core limit, that the crystal retains its structure in all but one of its cells, where it is broken. The broken cell corresponds to an exotic kind of repulsively bound state, which becomes delocalized. We investigate the excitation spectrum of the system analytically and find that the bound state behaves as a single particle hopping on an effective lattice with reduced periodicity, and is therefore gapless. Thus, the addition of a single particle to a flat-band system at critical filling is found to be enough to make kinetic behavior manifest.

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I. INTRODUCTION

Flat-band lattices, that is, lattices with a large degenerate subspace of single-particle solutions, have been the subject of interest for some time. For instance, they play a key role in the theory of ferromagnetism, where rigorous results by Lieb [1], Mielke [2], and Tasaki [3] guarantee the occurrence of ferromagnetism in flat-band Hubbard models, without the need for unrealistic long-range hopping terms. Also, the analogy between flat bands and the Landau levels enables the use of ultracold atomic systems [4,5] as a means of experimenting with quantum Hall physics [6–8]. The interface between flat-band ferromagnetism and topological band theory has also been studied [9–11]. The above examples pertain to fermionic systems, which are the main target of study in condensed matter physics. On the other hand, it is possible to engineer flat-band lattices for ultracold *bosons* by loading bosonic atoms into optical lattices [4,12]. Such systems are interesting in their own right, as they can be expected to support novel phases of matter not necessarily related to the quantum Hall effect or any other paradigmatic condensed matter phenomenon [13,14].

A flat band is simply an energy band in which the energy is constant, i.e., independent of the particle's quasimomentum. In a flat band, kinetic energy is an irrelevancy and behavior is governed entirely by interactions, so that even weakly interacting particles in the low-density limit enter a state that is strongly correlated and profoundly nonperturbative. Often, a consequence of such prepotency of interactions over kinetic terms is a Wigner-crystal-like ground state, in which the particles occupy nonoverlapping localized eigenstates [3,15–18]. In the repulsively interacting regime, and when the flat band is the band of lowest energy, this behavior can be explained via a simple energetic argument. It is energetically unfavorable for particles to overlap, but occupying a superposition of orthogonal flat band modes which is zero over all but a few lattice sites incurs no energy penalty. The system can avoid the energy cost of double and higher occupancies by filling the lattice with nonoverlapping localized eigenstates, and in this manner a crystal is formed. This picture, however, only holds true at low density. Above a critical filling factor ν_c ($\nu = N/L$ where N is the number of particles and L the number of lattice sites) there is insufficient space for every particle to occupy a localized state without any overlap, and the pure crystalline structure must be (at least partially) destroyed. The behavior of such lattice models at slightly above ν_c has been studied recently by Huber and co-workers in [13,19], and by Möller and Cooper [18]. In these works, the authors treat the weak-coupling limit, with the band gap much larger than the on-site interaction. They therefore assume that the ground state can be constructed entirely from (a projection onto) flat-band modes: an entirely justifiable approach, which provides excellent agreement with full-blown numerical calculations [13]. However, if the interaction energy is much larger than the band gap, the particles cannot all be expected to stay in superpositions of flat band modes as in the weak-coupling regime, and it is unclear how states which have contributions from the upper bands enter the problem, and how kinetic behavior, if at all, manifests.

Here we investigate strongly interacting bosons on a lattice supporting a flat lowest band. Specifically, we study the particularly simple sawtooth lattice (see Fig. 1), whose behavior above the critical filling fraction is understood in the weakly interacting regime [13] and has been the subject of study in the hard-core limit [20]. By investigating the situation where the filling fraction is $\nu = \nu_c + \epsilon$, with $\epsilon = O(1/N)$, we find that kinetic behavior does indeed occur at a filling slightly above the critical value, in the following, and rather unexpected, way. A two-body bound state is formed in the hard-core limit: a surprising result, given that the bosons comprising it do not overlap with each other. This bound state traverses the crystal as if it were a single particle acting under a pure hopping Hamiltonian, and moves with a quadratic dispersion relation at low energies, in stark contrast to the situation at and below critical filling where kinetic energy is completely quenched. Repulsively bound pairs in the Hubbard model have been studied [21–25] and observed

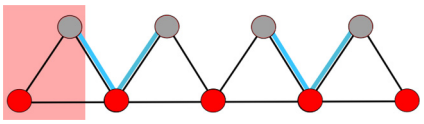

FIG. 1. (Color online) The sawtooth lattice, with a unit cell highlighted. A flat band occurs when the hopping amplitude between red sites is 1, and from red to grey is $\sqrt{2}$. The localized states associated with this band are shown in blue.

with ultracold atoms in optical lattices [26] and nonlinear optical systems [27], but the physical situations treated in those studies and experiments are completely different from the scenario analyzed here. For instance, in the above works the repulsively bound pairs exhibit large double occupancies for strong on-site interactions. By contrast, our result shows that it is possible to find repulsively bound pairs, *in the medium*, even when the particles are completely forbidden from overlapping. We note also that liquids of bound pairs have been found theoretically on the flat-band Creutz ladder in the weak-coupling limit [19,28].

II. SAWTOOTH LATTICE BELOW CRITICAL FILLING

The sawtooth lattice is effectively one dimensional (1D), being essentially a 1D chain with nearest- and next-nearest-neighbor hopping. For simplicity, and because we have in mind bosonic atoms in an optical lattice for the experimental realization, we model the system's dynamics by the Bose-Hubbard Hamiltonian with on-site interaction U,

$$H = \sum_{i,j} t_{i,j} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1), \tag{1}$$

where b_i ($b_i^\dagger$) is the bosonic annihilation (creation) operator at site i, $n_i = b_i^\dagger b_i$ is the number operator at site i, and where t_{ij} are hopping constants, given by

$$t_{2m,j} = t(\delta_{|2m-j|,2} + \sqrt{2}\delta_{|2m-j|,1}), \tag{2}$$

$$t_{2m+1,j} = t\delta_{|2m+1-j|,1}, \tag{3}$$

where m is an integer, and $t > 0$ is the nearest-neighbor tunneling rate. Note that we assume periodic boundary conditions, an even number of lattice sites, and have set the lattice constant to unity. To confirm that our choices for the t_{ij} do indeed give rise to a flat band, the single-particle problem must be solved. One may pass to first quantization and write the stationary Schrödinger equation $H\psi = E\psi$ as

$$\sum_{\mu=\pm1} t\left[\sqrt{2}\psi(j+\mu) + \frac{(1+(-1)^j)}{2}\psi(j+2\mu)\right] = E\psi(j). \tag{4}$$

Using Bloch's theorem to write the wave function as $\psi_k(j) = \phi_k(j)e^{ikj}$, where the $\phi_k(x)$ are functions of periodicity 2, gives two coupled equations,

$$E\phi_k(1) = 2t\sqrt{2}\cos 2k\, \phi_k(0) \tag{5}$$

$$(E - 2t\cos 2k)\phi_k(0) = 2t\sqrt{2}\cos k\, \phi_k(1). \tag{6}$$

This system is easily solved for the energy E, revealing the lowest flat and the excited dispersive bands,

$$E_0(k) = -2t, \tag{7}$$

$$E_1(k) = 2t(1 + \cos 2k). \tag{8}$$

The (unnormalized) localized eigenstates associated with the flat band (see [3] for mathematical details on the relationship between flat bands and localized states) are given by

$$V_i^\dagger|0\rangle = (\sqrt{2}b_{2i}^\dagger - b_{2i+1}^\dagger - b_{2i-1}^\dagger)|0\rangle. \tag{9}$$

It is easy to check that $HV_i^\dagger|0\rangle = E_0 V_i^\dagger|0\rangle$, from which one immediately concludes that the $V_i^\dagger|0\rangle$ are indeed superpositions of orthogonal flat band modes. Clearly, at most $L/4$ of these states can fit on the lattice without overlapping. Thus, up to $\nu = \nu_c = 1/4$, the (not necessarily orthogonal) degenerate many body ground states take the form

$$|\psi_0\rangle = \prod V_i^\dagger|0\rangle \tag{10}$$

where the product is over a set of N integers $\{i_1, i_2, \ldots, i_N : |i_m - i_n| > 1\ \forall m,n\}$. In what follows we take the hard-core limit $U \to \infty$, and thus allow at most one particle per site.

III. SCALING OF THE GROUND STATE ENERGY WITH SYSTEM SIZE

We now attempt to treat the sawtooth lattice at a single particle above critical filling. There are two ways of doing so without changing the periodic properties of the system: one may either add one particle on top of the preexisting $N = L/4$ (equivalent to reducing the size of the lattice by four sites), or remove one unit cell (two sites) from the lattice. We choose the latter option which is the simpler since, in the language of [13], it creates a single domain wall, as opposed to the former, which creates two. We have already pointed out the inadequacy of perturbative methods, so we adopt a variational approach. Thus our primary task is to decide upon a sensible ansatz. To this end, note that there are two ways in which the crystal phase might be destroyed: (*i*) the extra particle may become delocalized and upset the structure of the entire crystal, or (*ii*) it may remain localized and break one or several cells of the crystal, leaving the rest intact. We were able to decide between these two scenarios with the help of numerical evidence from exact diagonalization (ED) with up to five particles and periodic boundary conditions and from density-matrix-renormalization group (DMRG) [29,30] with up to 25 particles and open boundary conditions. In Fig. 2, we have plotted $C(N) = E(N) + (N-2)2t$. The quantity C represents the difference between the total ground state energy of the system and the energy of $N-2$ particles in nonoverlapping flat-band states. Thus, it can be viewed as the energy of an interacting two-body subsystem, if in the limit of $N \to \infty$ we have $E(N+1) - E(N) = C(N+1) - C(N) \to -2t$. ED shows that the change in the ground state energy tends very quickly to $E(N+1) - E(N) = -2t$ as N increases. For five bosons, the energy difference is already well converged, and we have $[E(5) - E(4)]/t = -2 - \mathcal{O}(10^{-4})$. DMRG reveals a similar trend, although the convergence is slower due to the open

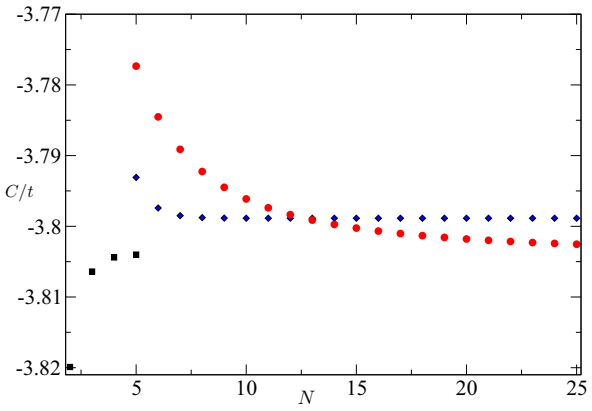

FIG. 2. (Color online) Comparison of energy obtained via minimization for various particle numbers (blue diamonds) with energies from DMRG (red circles) and exact diagonalization for five particles (black squares).

boundary conditions. This energy scaling strongly suggests that when an additional particle and four extra sites are added to the system at one particle above critical filling in the limit of a large lattice, the extra particle occupies a localized state. This leads us to postulate that when two lattice sites are removed from the critically filled lattice, $N-2$ of the localized states remain intact. The remaining two particles must avoid disrupting the localized states, and are thus confined to a block seven sites long. Since, when contributions from localized flat-band states are neglected, the ground state energy is close to that of two particles confined to seven sites with open boundary conditions, it seems natural to fill the seven-site block with its two-body ground state when we construct the ansatz.

IV. THE TRIAL WAVE FUNCTION

Denote a state in which the disrupted block begins on the $2i$th site as $|\psi_i\rangle$ (see Fig. 3), so

$$|\psi_i\rangle = B_i^\dagger \prod_{l=1}^{N-2} V_{i+2l+2}^\dagger |0\rangle, \tag{11}$$

where $B_i^\dagger = \sum_{j=0}^{5}\sum_{k=j+1}^{6} \alpha_{jk} b_{2i+j}^\dagger b_{2i+k}^\dagger$. The α_{jk} are chosen so that $B_i^\dagger|0\rangle$ is the ground state of a system of two particles in seven sites with open boundary conditions. Hence, we can write

$$H B_i^\dagger|0\rangle = E_B B_i^\dagger|0\rangle + X_i^\dagger|0\rangle, \tag{12}$$

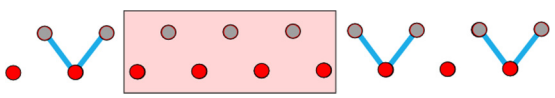

FIG. 3. (Color online) A pictorial representation of a component of the ansatz. The localized states are shown in blue. The highlighted block contains two particles and is diagonalized numerically. The full ansatz is a superposition of states like this, with the highlighted block starting on each red site.

where E_B is the seven-site ground state energy and $X_i^\dagger$ creates the terms that "leak" out from the disrupted block when the Hamiltonian is applied:

$$X_i^\dagger = \sum_{j=0}^{5} \alpha_{j6} b_{2i+j}^\dagger (\sqrt{2} b_{2i+7}^\dagger + b_{2i+8}^\dagger) + \sum_{j=1}^{6} \alpha_{j0} b_{2i+j}^\dagger (\sqrt{2} b_{2i-1}^\dagger + b_{2i-2}^\dagger). \tag{13}$$

Because of translational invariance, no particular block can be expected to contain the two-body state. Accordingly, our ansatz should be some superposition of the $|\psi_i\rangle$: $|\Psi\rangle = \sum_i \beta_i |\psi_i\rangle$. This last is our ansatz, with which we seek to minimize the energy expectation value, using the (complex-valued) β_i as variational parameters. We must solve

$$\frac{\delta}{\delta \beta_i^*}(\langle\Psi|H|\Psi\rangle - E\langle\Psi|\Psi\rangle) = 0, \tag{14}$$

where E is a Lagrange multiplier to be identified with the variational energies. After simple manipulation, Eq. (14) becomes

$$(C - E_B)\sum_j \langle\psi_i|\psi_j\rangle\beta_j = \sum_j \langle\psi_i|X_j^\dagger|0\rangle\beta_j \tag{15}$$

with $C = E - (N-2)E_0$. Notice that, since the states $|\psi_i\rangle$ are not orthogonal to each other, the above equation represents a generalized eigenvalue problem (GEP). The lowest value of C obtained by solving this GEP numerically for 25 particles agrees very well with the ground state value obtained via DMRG, which confirms that our ansatz is indeed a sensible one, and that the solutions of Eq. (15) furnish a good approximation to the set of exact eigenstates. See Fig. 2 for a comparison of the C obtained from functional minimization with that from DMRG.[1]

V. RESULTS AND DISCUSSION

Of course, Eq. (15) has $L/2$ solutions. The lowest energy solution is unique, and each subsequent solution is twofold degenerate, suggesting the existence of a quasimomentum-like quantum number. Each solution yields a set of β_j. Acting on our intuition about the quasimomentum, we label each set by an integer n, and have the energy increase monotonically with $|n|$. We let n run from $-L/4$ to $L/4-1$. The degenerate states are labeled $n = \pm|n|$, and the unique ground state has $n = 0$. With this labeling scheme, if k is defined as $k = 2\pi n/L$, we have verified numerically that $\beta_j^{(n)} = (-1)^{jn} e^{ijk}$ to machine accuracy, so

$$|\Psi_n\rangle = \sum_j (-1)^{jn} e^{ijk} |\psi_j\rangle. \tag{16}$$

[1] C, rather than E, is the pertinent quantity when it comes to assessing the accuracy of results here, since for any large value of N, the breakage energy, being of $\mathcal{O}(1)$, will be washed out by the trivial contribution of $\mathcal{O}(N)$ from the localized states.

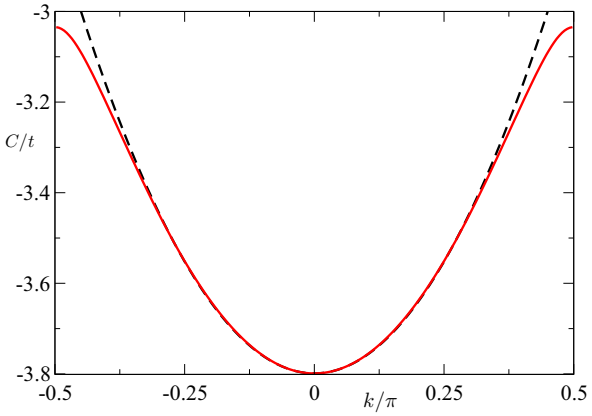

FIG. 4. (Color online) Dispersion relation for the moving bound state (solid red line), together with a quadratic function representing the dispersion of a free particle of mass $m^*/t = 1.25$ (dashed black line)

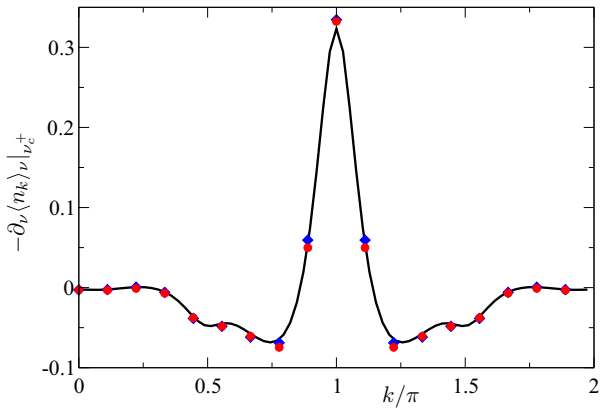

FIG. 5. (Color online) *Minus* the right derivative of momentum density as a function of filling fraction at critical filling, as per Eq. (17), as obtained from our ansatz with 20 particles (black line), five particles (blue diamonds) and from exact diagonalization with five particles (red circles).

The solution is equivalent to that of a single particle hopping on a lattice of periodicity 2, with Bloch functions $\phi_n(j) = (-1)^{jn}$, and the repulsively bound state playing the role of the particle. The dispersion relation is plotted in Fig. 4. It is exactly quadratic in the low energy sector, with an effective mass of approximately $m^*/t = 1.25$. The effective mass is apparently very large, as it is $\sim$10 times higher than the single-particle effective mass in the dispersive band $E_1(k)$, Eq. (8). However, if we compare this to the effective mass of the excitations in the weak-coupling limit, which is of $\mathcal{O}(t^2/U) \to \infty$ [13], we find that the effective mass is exceptionally low and therefore the contribution from the excited band is highly relevant. At low energies, then, there is a close analogy between our system at $N = N_c + 1$ and a (heavy) single free particle in the continuum.

Our predictions can be verified experimentally by measuring the ground state momentum distribution, an experiment that is routinely performed with ultracold atoms in optical lattices [31–33]. We now calculate the expected results, and while doing so demonstrate nonanalytic behavior—an instability—around critical filling. At $\nu \leqslant \nu_c$, it is a simple matter to show that

$$\langle n_k \rangle_{\nu \leqslant \nu_c} \equiv \langle \psi_0 | n_k | \psi_0 \rangle = \frac{\nu}{4}(\sqrt{2} - \cos k)^2. \qquad (17)$$

At $\nu = \nu_c + \epsilon$ the momentum density deviates from Eq. (17) slightly. This deviation is due to the addition of a single particle and hence rather small, so a direct measurement of $\langle n_k \rangle_{\nu_c}$ is unlikely to give usable data. Rather, measuring $\langle n_k \rangle_{\nu_c \pm \epsilon}$ and $\langle n_k \rangle_{\nu_c}$, and thence calculating the right derivative,

$$\frac{\langle n_k \rangle_{\nu_c+\epsilon} - \langle n_k \rangle_{\nu_c}}{\epsilon} = \left.\frac{\partial \langle n_k \rangle}{\partial \nu}\right|_{\nu_c^+} + \mathcal{O}(\epsilon), \qquad (18)$$

would yield data that can be meaningfully compa red with the derivative obtained from our model, shown in Fig. 5. It is clear from Eq. (17) and Fig. 5 that the right and left derivatives do not agree at ν_c; this singularity is a signature of the destruction of the crystalline structure.

Since a variational estimate of the ground state energy is only approximate, we must rule out the existence of states with a lower energy than, and different nature from, our ansatz. Firstly, the nontrivial contribution, C, to the ground state energy obtained variationally in the large N limit differs by only 0.1% from the well-converged ED result with five particles, which is a remarkable degree of agreement. Moreover, the right derivative of the momentum distribution obtained from our model is in excellent agreement with results from ED, and reproduces its oscillatory and peak structure very well. Moreover, since our variational treatment is computationally inexpensive, we are able to calculate the momentum distribution in the large N limit (see solid line in Fig. 5). The fact that all the qualitative and quantitative features of the derivative throughout the Brillouin zone are captured by our ansatz shows that the ground state is very closely related to the one we propose: a lower energy may be reachable by allowing more free parameters, but the fact that the overall ground state is a repulsively bound pair confined to a small block within a medium of localized flat band states is indisputable.

We also compare the excitation spectrum generated by the ansatz with results from ED with five particles (Fig. 6) and find an encouraging degree of agreement in the low-energy sector, where the ansatz is reliable (it becomes unreliable at higher energies due to, for instance, the possible existence of internal excitations of the bound state).

In summary, although kinetic energy is quenched at ν_c or below, we find that an extra particle above ν_c does away with this quenching: the interaction is no longer the only relevent parameter.

Kinetic behavior manifests in the form of a novel repulsively bound pair traveling through the lattice. The emergence of kinetic behavior and the existence of this nonoverlapping repulsively bound state are our main findings.

The fact that the excitation spectrum is gapless leads us to believe that we have found the lowest lying states, and this, together with the closeness between our groundstate energy and the DMRG result and the agreement on the momentum distribution between exact diagonalization and our model,

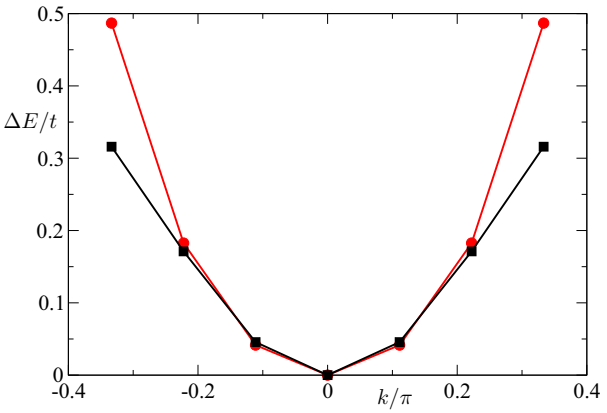

FIG. 6. (Color online) Comparison of the excitation spectrum with respect to the ground state energy generated by the ansatz (red circles) with that from exact diagonalization (black squares) for five particles.

suggests that we have captured all the essential low-energy physics with our picture.

VI. FUTURE WORK AND OUTLOOK

The single-particle-like nature of solutions at $N = N_c + 1$ indicates to us the possibilty of modeling behavior at a few particles above N_c via a theory (perhaps exactly solvable) of interacting bound states. Further, we suspect that our findings are not limited in their applicability to the sawtooth lattice, and give insight into the general nature of the destruction of lattice Wigner-like crystals by overfilling. A confirmation or refutation of this suspicion would be interesting; were it to be confirmed, we would have a general prescription for treating flat-band lattice models above ν_c.

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