On-site correlations in optical lattices: band mixing to coupled quantum Hall puddles

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We extend the standard Bose-Hubbard model to capture arbitrarily strong on-site correlations. In addition to being important for quantitatively modeling experiments, for example, with Rubidium atoms, these correlations must be included to describe more exotic situations. Two such examples are when the interactions are made large via a Feshbach resonance, or when each site rotates rapidly, making a coupled array of quantum Hall puddles. Remarkably, even the mean field approximation to our model includes all on-site correlations. We describe how these on-site correlations manifest themselves in the system’s global properties: modifying the phase diagram and depleting the condensate.

Optical lattice systems, where a dilute atomic gas is trapped in a periodic potential formed by interfering laser beams, provide a close connection between solid state systems and atomic physics [1]. The models used to describe these systems generally assume that each lattice site’s wavefunction is easily built up from single particle states [2]. Here we argue that this approximation is inappropriate to quantitatively model current experiments, and sometimes fails more drastically, e.g., for resonant bosons. We show how to include arbitrary on-site correlations via a generalized Hubbard model, which can be approached by standard methods. By construction, the mean field approximation to our model captures all on-site correlations.

Our method’s key idea is to first consider deep lattices, where lattice sites are isolated and then solve the few-body problem on each site. Next, truncating to this few-body problem’s low energy manifold, we calculate few-body problem on each site. Next, truncating to this few-body problem’s low energy manifold, we calculate on-site correlations. The principle difference is that states defined in this way are non-orthogonal. From these, however, one can construct a new set of orthogonal states. The number of excited states is straightforward. Note that even in the non-interacting case these states are non-orthogonal. F rom these, however, one can construct a new set of orthogonal states |\psi_j\rangle, which hold similar physical meaning. In the noninteracting limit, the |\psi_j\rangle approximate the Wannier states.

Because the single-site wavefunctions decay like Gaussians, it typically suffices to build up the effective Hamiltonian from neighboring sites. In particular, consider two sites L and R, and the space spanned by |n_L, n_R\rangle = |n_L\rangle_L \otimes |n_R\rangle_R, with overlaps S^{(mn)} = \langle m, n | m + 1, n - 1 \rangle. To lowest order in the overlaps, we can define orthogonal |n_L, n_R\rangle by taking |n_L, n_R\rangle = |n_L, n_R\rangle - (1/2) |S^{(n_L, n_R)}| |n_R + 1, n_L - 1 \rangle + S^{(n_L, n_R)}| |n_R - 1, n_L + 1 \rangle.

Within this restricted basis, the effective Hamiltonian for these two sites is H_{eff} = \sum_{n, m, n', m'} |\psi_j, m\rangle \langle n, m | H_f | n, m \rangle \langle n, m |. Evaluation to lowest order in S^{(mn)} yields on-site energy terms

\sum_{n, m} \langle n, m | H_f | n, m \rangle \langle n, m | + H.c.

with H_{cell} = \langle n | H_f | n \rangle

\langle n | H_f | n \rangle = -\langle m + 1, n - 1 | H_f | m, n \rangle + \frac{S^{(mn)}}{2} (E_m + E_n) + H.c.

Additionally there is an interaction term U =
\[ \sum_{nm} [U^{n}(m) + U^{m}(n)] \langle m, n | = U_{LL}^{(m)} = E_m \quad \text{and} \quad U^{(n,m)}_{LR} = \langle m, n | H | m, n \rangle - E_m - E_n \quad (3) \]

to \( O(S^2) \), consistent with the rest of our calculations. In the remainder of this paper we will neglect the off-site interaction, Eq. [3], and the last term in Eq. [2]. The former is rigorously justified as it falls of exponentially faster than the other interaction terms. Formally, the non-orthogonality contribution to Eq. [2] is suppressed only by a factor of \( (V_0/E_R)^{1/4} \) with \( E_R = \hbar^2 \pi^2 / (2md^2) \), but as shown in Fig. 1 it is typically small.

The simplest many-site Hamiltonian which reduces to this one in the limit of two sites is

\[ H = - \sum_{i,j,\sigma} t^{(i,j)}_{\sigma} | i \rangle \langle i | \sigma \rangle + \frac{1}{2} \sum_{i,n} E_n \left| \sum_j \right| \langle i | \langle n | j \rangle \langle n | j \rangle + \sum_{i,n} E_n | i \rangle \langle i | n \rangle \langle n | i \rangle , \quad (4) \]

where \( \sum_{i,j} \) indicates a sum over nearest neighbors \( i \) and \( j \). At higher order, one generates more terms such as next nearest neighbor hoppings, pair hoppings, and longer range interactions.

Calculating the Hamiltonian parameters.—Here we consider the cases of weak interactions, resonant interactions, and coupled quantum Hall puddles.

In the limit of weak interactions, one can estimate the parameters in Eq. [4] by taking the on-site wavefunction to be \( \psi_n \propto \exp(-\sum_{j=1}^{n} r_j^2/2\sigma_n^2) \), with variational width \( \sigma_n \). To leading order in \( a/d \) we find \( E_n = E_R \left[ 3\sqrt{V_0/E_R} - \mu/E_R n \right] + U n(n-1) \left[ 1 - \frac{3}{4\sqrt{\pi}} (a/d)(n-1)(V_0/E_R)^{1/4} \right] \) with \( U = (a/d)\sqrt{2\pi}(V_0/E_R)^{3/4} \) and \( t^{(mn)} = t^{(nn)} = t^{(m+1)} = \sqrt{n(m+1)}[1 + \sqrt{2\pi} \frac{1}{2d}(m + n - 1)(V_0/E_R)^{3/4}] \) with \( t = V_0(\pi/4 - 1)e^{-n^2/4}/\sqrt{V_0/E_R} \). Note that as expected, interaction spreads out the Wannier functions, increasing the \( t^{(nn)} \)’s and decreasing the \( E_n \)’s. Fig. 4 shows several of the resulting \( t^{(nn)} \) as a function of \( V_0 \) for parameters in typical optical lattice experiments with \( ^{87}\text{Rb} \). Also shown are \( t^{(01)} \) and the next-nearest-neighbor hopping, \( t_{nnn} \), calculated from the exact Wannier states. Our estimates are consistent with previous work regarding \( t \)-dependence \( [3, 4, 14] \), validating our approach. As can be seen in Fig. 1(c), the relative size of the nearest neighbor hopping \( t_{nnn}/t \) is 10% (1%) for \( V_0 = 3E_R \) (\( V_0 = 10E_R \)), justifying our approximation of including only nearest neighbor overlaps to describe the system near the Mott state. We also see that even for this weakly interacting case the number dependence of \( t \) is crucial for a quantitative description of the experiments. Similarly, the number dependence of the on-site interaction is quantitatively significant. This latter deficiency of the standard Hubbard model has been noted in the past, for example by the MIT experimental group \[ 14].

For more general experimental systems, one needs to include still more on-site correlations. As our first example, we consider lattice bosons near a Feshbach resonance \[ 12, 13 \], describing, for example, ongoing Cesium atom experiments \[ 3 \]. We restrict ourselves to site occupations \( n = 0, 1, 2 \), for which we have exact analytic solutions to the on-site problem for arbitrary \( a \) in terms of confluent hypergeometric functions \[ 14 \]. Fig. 2 shows graphs of \( E_n \) and \( t^{(nn)} \) recasted by \( \hbar \omega \) as a function of \( a \) in the deep lattice limit.

As Fig. 2(b) illustrates dramatically, the hopping from and to doubly-occupied sites is strongly suppressed near the Feshbach resonance when atoms occupy the lowest branch, and is enhanced for the next-lowest branch. The former has implications for studies of boson pairing on a lattice \[ 12, 13 \], showing that one must dramatically modify previous models near resonance, and, as will be discussed more below, the latter implies a substantial reduction of the \( n = 2 \) Mott lobe’s size for repulsive bosons.

We give one further example, namely the case, similar to the one discussed in \[ 4, 5 \], where the individual sites of the optical lattice are elliptically deformed and rotated about their center. This is accomplished by rapidly modulating the phase of the optical lattice lasers to generate an appropriate time-averaged optical potential. At an appropriate rotation speed \( \Omega \) the lowest energy \( n \)-particle state on each site is a \( \nu = 2 \) Laughlin state \( \psi_n(\mathbf{r}_1, \ldots \mathbf{r}_n) = N_n \prod_{i<j=1}^{n} (w_i - w_j)^2 \phi(\mathbf{r}_1, \ldots \mathbf{r}_n) \), where we define \( w_j = x_j + iy_j \), and \( N_n \) is a normalization factor with phase chosen to gauge away phase factors appearing in \( t^{(mm)} \). Truncating to this set of states for
n = 0, 1, 2, we produce an effective Hubbard model of the same form as Eq. (4). The hopping parameters for asymptotically deep lattices V_0/E_R ≫ 1 are \(t^{(01)} = t\), \(t^{(02)} = t(\pi^2/32)/(V_0/E_R)^{1/2}\), and \(t^{(12)} = t(\pi^4/1024)/(V_0/E_R)\), where \(E_R = h^2\pi^2/(2md^2)\) is the recoil energy, and \(t\) is the same as in the weakly interacting case treated above; the interaction parameters are \(E_m = \frac{d}{a}m(n-1) - \mu n\). One particularly interesting aspect of this model of coupled quantum Hall puddles is that when the system is superfluid, the order parameter is exactly the quantity defined by Girvin and MacDonald \(\bar{\epsilon}_{m+n}^c\) to describe the nonlocal order of a fractional quantum Hall state. Thus when one probes the superfluid phase stiffness, one directly couples to this quantity.

**Mean-field theory.**—The true strength of our approach is that the resulting generalized Hubbard model is amenable to all of the analysis used to study the standard Bose-Hubbard model. In particular, we can gain insight from a Gutwiler mean-field theory (GMFT) \(\Omega\). This approximation to the ordinary Bose-Hubbard model gives moderate quantitative agreement with more sophisticated methods: for example, the unity site filling MI/SF transition on a 3D cubic lattice occurs at \(\langle t/U \rangle_c = 0.03408(2)\) while GMFT yields \(\langle t/U \rangle_c = 0.029\) \(\Omega\).

In the ground state \(|\Psi\rangle\), we introduce mean fields \(\zeta_m ≡ \langle \Psi | m+1 \rangle | m \rangle\). Neglecting terms which are quadratic in \(\delta L'_{m} = | i, m + 1 \rangle \langle i, m | - \xi_m\), the Hamiltonian is \(H_{MF} = \sum_i H_{MF,i}\) with

\[
H_{MF,i} = E_{n_i} | n_i \rangle \langle n_i | - z \sum_m \left[ \zeta_m | m-1 \rangle \langle m | - \zeta_m \xi_{m+1} + \text{H.c.} \right],
\]

where \text{H.c.} denotes Hermitian conjugate, \(z\) is the lattice coordination number, and \(\zeta_n = \sum_m \zeta_m | m \rangle | m \rangle\).

Truncating the number of atoms on a site to \(n ≤ n_{\text{max}}\), we self-consistently solve Eq. (5) by an iterative method. We start with trial mean-fields, calculate the lowest energy eigenvector of the \((n_{\text{max}}+1) \times (n_{\text{max}}+1)\) mean field Hamiltonian matrix, then update the mean-fields. We find that it typically suffices to take \(n_{\text{max}}\) roughly three times the mean occupation of the sites. Fig. 3 illustrates how the density dependence of the parameters introduced by the on-site correlations modify the GMFT phase diagram — particularly the phase boundary’s shape, and the density and order parameter in the superfluid phase.

As one would expect, the topology of the MI/SF phase boundaries are similar to that of the standard Bose-Hubbard model, but the Mott lobes’ shapes can be significantly distorted. Within mean-field theory the boundary’s shape can be determined analytically by taking \(|\Psi\rangle = \epsilon | n+1 \rangle + \sqrt{1 - \epsilon^2} f_{n-1} | n \rangle + \epsilon | n \rangle|\), and expanding \(\langle \Psi | H_{MF} | \Psi \rangle\) to quadratic order in \(\epsilon\) and \(\epsilon^\prime\). The Mott boundary corresponds to when the energy expectation value’s Hessian changes sign; this boundary oc-

![FIG. 2: (color online) Left: On-site two-particle energy as a function of scattering length \(a\) rescaled by the on-site harmonic oscillator energy \(\hbar \omega = 2 \sqrt{V_0 E_R}\), for the two lowest energy branches. The corresponding characteristic length is \(\ell = \sqrt{\hbar/\omega}\). Right: Log plot of rescaled hopping matrix elements \(\ell^{(1)}(\sqrt{m+1})/|t^{(1)}(\sqrt{m+1})|\). Solid and dashed curves are \(\ell^{(1)}/(\sqrt{2t})\) and \(\ell^{(2)}/(2t)\), respectively. We have chosen the lattice depth \(V_0 = 15 E_R\); this affects only the horizontal scale. In the ordinary Bose-Hubbard model, \(\ell^{(1)}(\sqrt{m+1})/|t^{(1)}(\sqrt{m+1})| = 1\) for all \(m, n\), as confirmed by this figure’s \(a = 0\) lowest branch and \(a = 0\) second branch limits. The resonance at \(-d/a = 0\) separates the molecular side (left), from the atomic side (right).](image)

![FIG. 3: (color online) Representative Gutwiler mean-field theory phase diagrams, showing constant density (black, roughly horizontal) and constant \(\xi = \zeta_1 + \zeta_2 + \zeta_3\) (red, roughly vertical) contours: \(\xi\), similar to the condensate density, is a combination of the mean fields \(\zeta_m\), defined after Eq. (4). Density contours are \(n = \{0.01, 0.2, 0.5, 0.8, 0.99, 1, 1.2, \ldots\}\) and order parameter contours are \(\xi = \{0.2, 0.4, \ldots\}\), except (d) where we take contours \(\xi = \{0.02, 0.04, \ldots\}\). The phase diagrams are functions of \(\mu_{\text{eff}} \equiv \mu/E_{\text{rec}}\) and \(t_{\text{eff}} \equiv \exp(-\sqrt{V_0/E_{\text{rec}}})\), where the lattice depth \(V_0\) is the natural experimental control parameter. We plot versus \(t_{\text{eff}}\), instead of \(V_0\), as this is closer to the Hamiltonian matrix elements and more analogous to traditional visualizations of the Bose-Hubbard phase diagram. (a) Ordinary Bose-Hubbard model for \(a = 0.01 d\), (b) resonant lattice bosons restricted to fillings \(n = 0.1, 2\) with \(a = 0.01 d\), on the next to lowest energy branch on the \(a > 0\) side of resonance, (c) resonant lattice boson model with \(a = d\), and (d) FQH puddle array model taking \(\omega - \Omega = 0.1 E_{\text{rec}}\) (see text for details).](image)
Finally, although we have truncated to a single many-body state for each filling \( n \), no difficulty arises from including on-site many-body excitations in the Hamiltonian. These are especially important, for example, for double well lattices and spinor bosons. The ideas also extend straightforwardly to fermions; see Refs. [21, 22] for related considerations.

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\( \bar{\mu} \equiv \frac{E_n - E_{n-1}}{E_n}, \quad x_U \equiv \frac{E_{n+1} + E_{n-1} - 2E_n}{E_n}, \)
\( \bar{t} \equiv \frac{t^{(n,n)}}{E_n}, \quad t^+ \equiv \frac{t^{(n,n+1)}}{t^{(n,n)}}, \quad t^- \equiv \frac{t^{(n-1,n)}}{t^{(n,n)}}. \)