Large effective three-body interaction in a double-well optical lattice

Saurabh Paul

Eite Tiesinga
Joint Quantum Institute
Joint Center for Quantum Information and Computer Science
University of Maryland, College Park

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Introduction

- Simulations of many-body systems with atoms in optical lattices.
- The goal is to create effective Hamiltonians with large three-body interactions.
- We use an optical lattice with two local minima per unit cell.
- This gives us a multi-band Bose-Hubbard (BH) Hamiltonian.
- We show that the low energy states of this Hamiltonian is equivalent to a single-band BH Hamiltonian with large effective three-body interaction energy, i.e.,

$$H_{\text{eff}} = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{1}{6}\Gamma_3 \sum_i b_i^\dagger b_i^\dagger b_i^\dagger b_i b_i b_i$$

where $b_i^\dagger$ creates a particle in unit cell i.

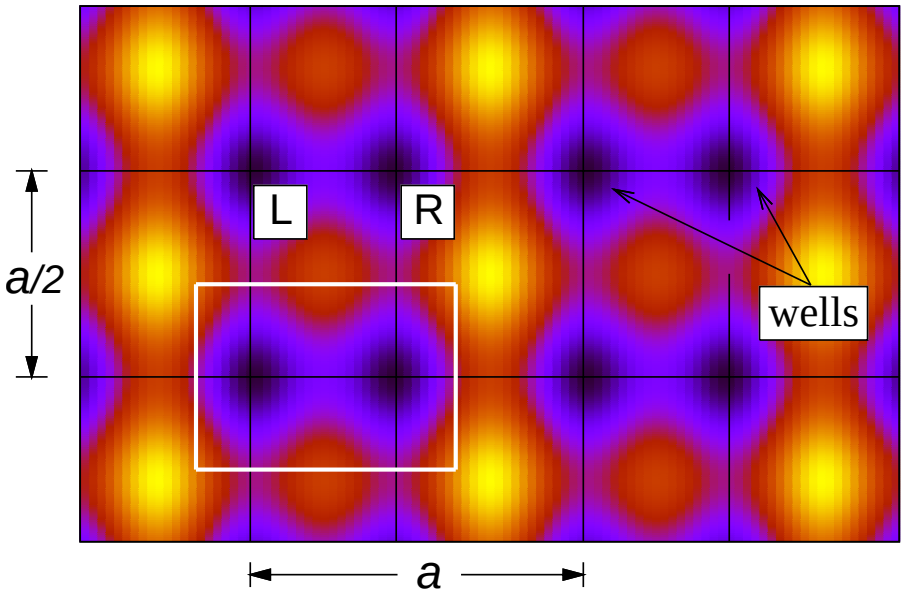
Optical lattice potential

- The mathematical form for the optical lattice potential is

$$V(x) = -V_0 \cos^2(k_L x) - V_1 \cos^2[2k_L(x + x_0)] - V_2 \left\{\cos^2(2k_L y) + \cos^2(2k_L z)\right\}.$$

- k_L is the laser wave vector.
- x_0 controls the lattice asymmetry.
- $k_L x_0 = \pi/4$ gives a symmetric lattice.
- The potential has three depths V_0, V_1 and V_2.
- V_1/V_0 controls the barrier height between the left and right wells within a double well.
- Typically, we use a symmetric lattice, vary the depth V_0 while keeping the ratio V_1/V_0 fixed.

Optical lattice potential...



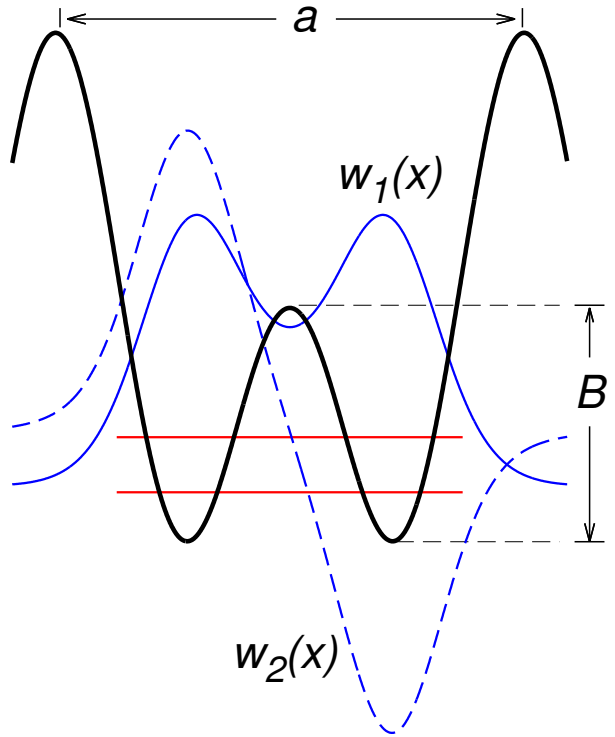


Figure : (a) Contour plot of the optical lattice potential in the xy plane. (b) Schematic of a symmetric double-well potential along the x axis, along with the localized Wannier functions $w_1(x)$ and $w_2(x)$ for the lowest two Bloch bands along the x direction.

Two-band BH Hamiltonian

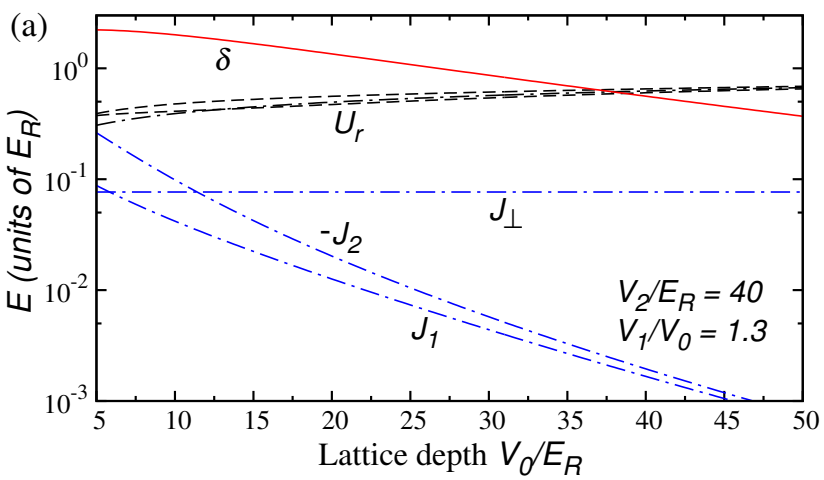
- We first set up a BH Hamiltonian for Wannier functions belonging to the two lowest bands. Other bands are energetically well separated.
- Hopping occurs only between nearest-neighbor unit cells.
  - J_1 is the hopping along the x axis in band one,
  - J_2 is the hopping along the x axis in band two,
  - $J_\perp$ is the hopping along the perpendicular y and z axes.
- Within a unit cell we have single- and two-atom terms
  - δ is the band-gap between the two lowest bands,
  - U_α is the two-body interaction strength for band $\alpha = 1, 2$,
  - U_{12} is the pair-wise interaction strengths between the bands.
- Crucially, we have a strong pair hopping term

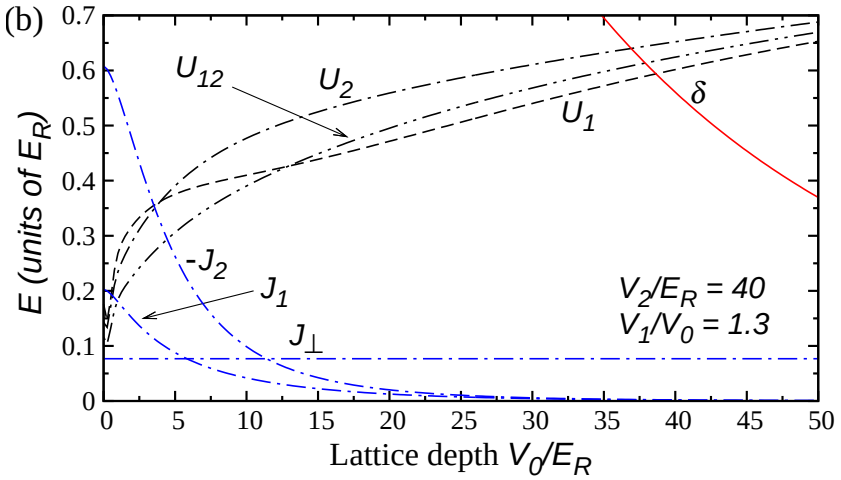
$$\frac{1}{2} U_{12} \left(a^\dagger_{\mathbf{i},1} a^\dagger_{\mathbf{i},1} a_{\mathbf{i},2} a_{\mathbf{i},2} + a^\dagger_{\mathbf{i},2} a^\dagger_{\mathbf{i},2} a_{\mathbf{i},1} a_{\mathbf{i},1} \right)$$

where $a^\dagger_{\mathbf{i},\alpha}$ creates a particle in the Wannier function of band α in unit cell $\mathbf{i}$.

BH Hamiltonian parameters

- We have determined numerically the seven parameters in our BH model as a function of the lattice depths V_0, V_1 and V_2.
- The figures show typical data vs V_0 for a symmetric double-well in units of the recoil energy E_R
- Panel (a): log-linear scale, Panel (b): linear-linear scale.





- The interaction energies are of similar strength and of the order of the band gap δ.
- The interaction energies are much larger than the tunneling energies.

Effective Hamiltonian

Constructing the effective Hamiltonian is a three-step process

1. Inspired by the smallness of the tunneling energies, diagonalize the on-site Hamiltonian in unit cell $\mathbf{i}$ to obtain many-particle (MP) energy levels.
2. Using these MP levels, construct an effective on-site interaction Hamiltonian in each unit cell.
3. Finally, calculate the effective tunneling Hamiltonian that couples the MP states of adjacent unit cells.

Many-particle energy levels

- The MP levels are obtained in terms of the Fock state basis

$$|\nu, N\rangle = \sum_{n_1=0}^{N} \mathcal{C}_{n_1}^{(\nu)}(N)|n_1, N-n_1\rangle, \quad \text{where} \quad \nu = \{1, \ldots, N+1\}.$$

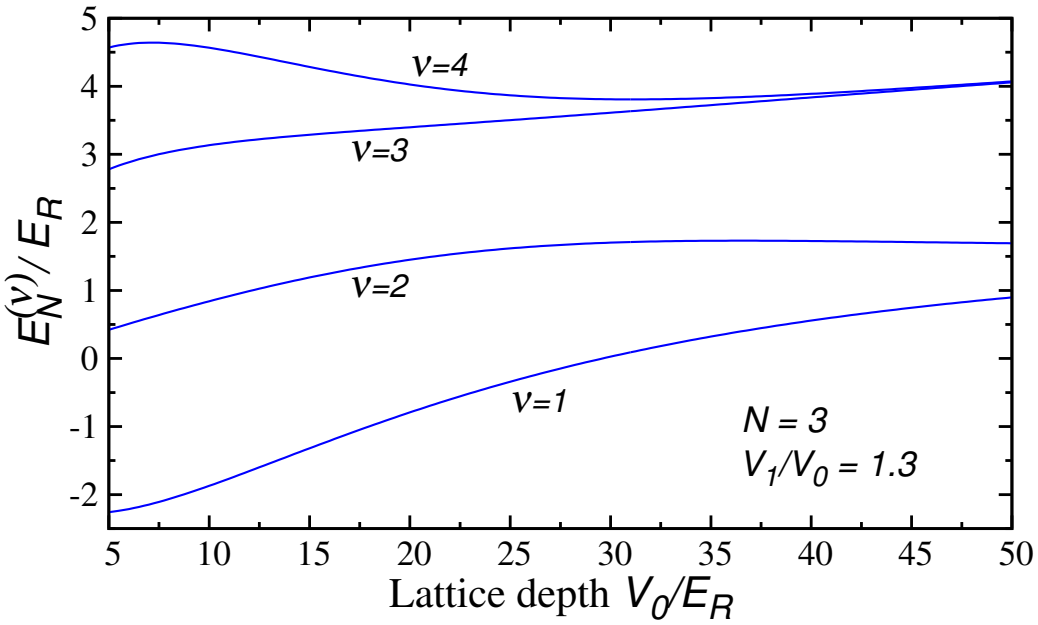
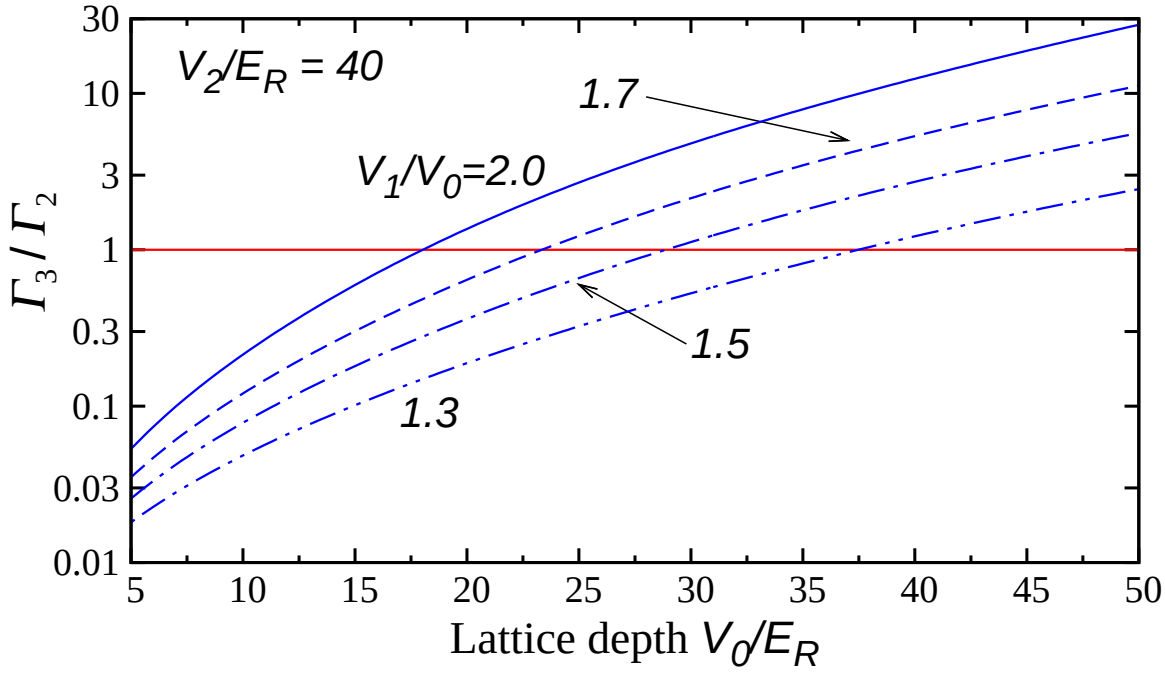


Figure : Plot of MP levels $\mathcal{E}_N^{(\nu)}$ for N = 3 atoms per unit cell.

- The energies of the ground vibrational states $\mathcal{E}_N^{(1)}$ are well separated from the excited state energy levels.

Effective interaction Hamiltonian



- Atoms only populate the ground vibrational $\nu = 1$ state.
- The energies $\mathcal{E}_N^{(1)}$ are reproduced by an effective on-site interaction Hamiltonian

$$H_{\text{eff}}^{\text{int}} = \sum_{\mathbf{i}} \sum_{m=1}^{3} \frac{1}{m!} \Gamma_m b_{\mathbf{i}}^{\dagger m} b_{\mathbf{i}}^{m}.$$

- $b_{\mathbf{i}}^{\dagger}$ creates a particle in unit cell $\mathbf{i}$ in the state $|\nu = 1, N\rangle$.

Effective tunneling Hamiltonian

- Predominant terms are the usual single-particle hopping terms.
- Followed by the density-induced two- and three-body terms which have the forms $J_{2b} b_i^\dagger (b_j^\dagger b_j) b_j$ and $J_{3b} b_i^\dagger (b_i^\dagger b_i b_j^\dagger b_j) b_j$, respectively. They, however, are small.
- Thus, tunneling surprisingly has the same structure as that for a particle hopping in a single-band BH model.
- Tunneling mainly occurs in the ground band. Excited band tunneling which is proportional to J_2 can be ignored.
- Tunneling mixes vibrational states. To a good approximation, we only include tunneling between the ground $\nu = 1$ states.
- The effective tunneling Hamiltonian is

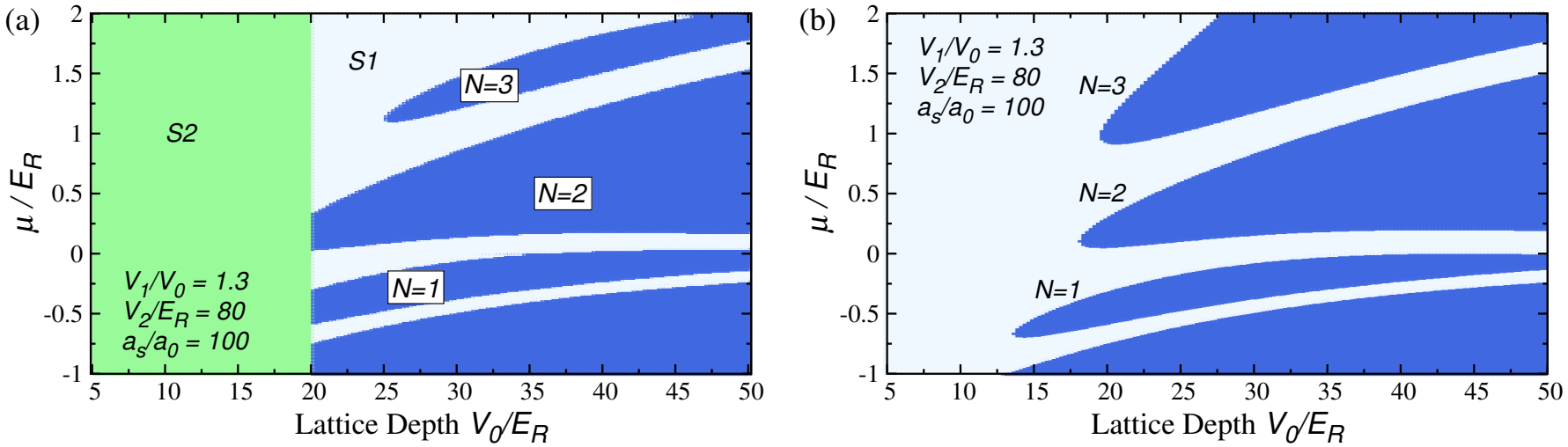
$$H_{\text{eff}}^{\text{hop}} = \sum_{\mathbf{i}} \left\{ -J_1 b_{\mathbf{i}}^\dagger b_{\mathbf{i}+1_x} - J_\perp \left(b_{\mathbf{i}}^\dagger b_{\mathbf{i}+1_y} + b_{\mathbf{i}}^\dagger b_{\mathbf{i}+1_z} \right) + h.c. \right\}.$$

Validity of the effective Hamiltonian

- The effective Hamiltonian is given by

$$H_{\text{eff}} = \sum_{\mathbf{i}} \left\{ \sum_{m=1}^{3} \frac{\Gamma_m}{m!} b_{\mathbf{i}}^{\dagger m} b_{\mathbf{i}}^{m} - J_1 b_{\mathbf{i}}^{\dagger} b_{\mathbf{i}+1_x} - J_\perp \left(b_{\mathbf{i}}^{\dagger} b_{\mathbf{i}+1_y} + b_{\mathbf{i}}^{\dagger} b_{\mathbf{i}+1_z} \right) + h.c. \right\}.$$

- Perform Mean-field calculation for SF-Mott phase diagram.
- Panel (a): Full Hamiltonian Panel (b): H_{eff}



- Cutting off of Mott lobes in Panel (a) at $J_2 + 2J_\perp = 0$.
- Of primary interest is SF region $S1$ where there is excellent agreement between full and effective Hamiltonians.

Conclusion

- The low energy states of a system of trapped atoms in a double-well optical lattice can emulate a Hubbard model with strong three-body interactions.
- The full Hamiltonian has a strong pair-tunneling term. The interplay between this term and the band gap largely determines the behavior of the system.
- The strength of the effective three-body interaction can be easily tuned by changing the lattice parameters.
- Surprisingly, tunneling in the effective Hamiltonian has, to good approximation, the same structure as that for a particle hopping in a single-band BH model.
- The effective Hamiltonian model is an excellent approximation over a wide range of lattice parameters, both in the superfluid and Mott insulator phases.