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# Effective three-body interactions in an asymmetric double-well optical lattice Saurabh Paul, Eite Tiesinga QuICS, National institute of Standards and Technology

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### Introduction

We study ultracold atoms in a double-well optical lattice, with a view to creating an effective Hamiltonian that has large threebody interaction energy. The Bose-Hubbard (BH) Hamiltonian for such a system spans the lowest two bands  $3E + U_{2}$ along x-axis, and the ground band along the perpendicular axes. We obtain the many-particle (MP) states, 3 particles  $|\nu, N\rangle, \nu \in \{1, N+1\},$  by diagonalizing the BH Hamiltonian in the particle number basis. These MP energy levels are shown in the schematic alongside. Using the  $\nu = 1$  state in each MP 2 particles sector, we create an effective Hamiltonian,  $H_{\rm eff} = \sum_{1}^{3} \frac{b^{\dagger m} b^{m}}{m!} \Gamma_{m},$ Esuch that the effective three-body 1 particle interaction energy is comparable to or larger than the two body term, i.e.,  $\Gamma_3 \gtrsim \Gamma_2$ . The ratio  $\Gamma_3 / \Gamma_2$ can be tuned by changing the lattice parameters.

#### Exact band structure calculation









Symmetric

The Wannier functions are obtained numerically from an exact band structure calculation. Figure (left) shows them for first two bands. Figure (right) shows the two-body interaction terms and tunneling energies numerically obtained using these functions.

#### Many particle energy (MPE) levels



The interaction part of the Hamiltonian H can be diagonalized in a particle number basis  $|n, N\rangle$ , where n is the atom number in ground band, and N is the number of atoms per lattice site. This

 $V(x) = -V_0 \cos^2(k_L x) - V_1 \cos^2[2k_L (x+b)].$ 

The lattice has asymmetric double-wells along the x axis (above), and single wells along the y & z axes. Tunneling elements,  $t \gg J > J_L \gtrsim J_R > J_{LR} > J_{RL}$ . Nearest-neighbor tunneling cannot be neglected! We are interested in nearly symmetric lattice, i.e.,  $k_L b \approx \pi/4$ .

Starting multiband Hamiltonian

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The starting point is the Hamiltonian for this system, which somewhat simplifies in the band basis, and along x axis is,  $H = \sum_{i} \left\{ \frac{\delta}{2} (a_{i,2}^{\dagger} a_{i,2} - a_{i,1}^{\dagger} a_{i,1}) + \frac{1}{2} \left( U_{1111} a_{i,1}^{\dagger} a_{i,1}^{\dagger} a_{i,1} - U_{2222} a_{i,2}^{\dagger} a_{i,2}^{\dagger} a_{i,2} a_{i,2} - a_{i,2}^{\dagger} a_{i,2} - a_{i,2}^{\dagger} a_{i,1} - U_{2222} a_{i,2}^{\dagger} a_{i,2} - a_{i,2}^{\dagger} a_{$  gives the many-particle energy eigen-states  $|\nu, N\rangle, \nu \in \{1, N+1\},\$ with energies  $\mathcal{E}_N^{\nu}$ . Figure (left) shows the two-particle energies for various double-well barrier heights. Figure (right) is a similar plot for the three-particle energies.

**Effective three-body interaction** 



The effective interactions can be expressed in terms of the MPEs,  $\Gamma_2 = \mathcal{E}_2 - 2\mathcal{E}_1$  and  $\Gamma_3 = \mathcal{E}_3 - 3(\mathcal{E}_2 - \mathcal{E}_1)$ . For large lattice depths, choosing only the ground states in each MP sector, we can show that,  $\Gamma_2 \approx \delta$  and  $\Gamma_3 \approx 2U_{1111} \approx 2U_{2222}$ . Thus, ratio  $\Gamma_3/\Gamma_2$ 

 $i + \frac{1}{2} U_{1122} \left( 4a_{i,1}^{\dagger} a_{i,1} a_{i,2}^{\dagger} a_{i,2} + a_{i,1}^{\dagger} a_{i,1}^{\dagger} a_{i,2} a_{i,2} + a_{i,2}^{\dagger} a_{i,2}^{\dagger} a_{i,1} a_{i,1} \right) \\ - \sum_{\alpha \in 1,2} J_{\alpha} \left( a_{i,\alpha}^{\dagger} a_{i+1,\alpha} + h.c. \right) \right\}$ 

where,  $\delta$  is the band gap between the two lowest bands. The various two-body interaction terms and tunneling energies are numerically obtained (section 4).

## Summary & Outlook

We have created an effective Hamiltonian picture to describe a system of ultracold atoms in a double-well potential. This effective Hamiltonian has large three-body interaction energies, which can be tuned by changing the lattice parameters. Also, the effective Hamiltonian in addition has density induced tunneling energy terms between adjacent sites. We are now looking at the possibility of having unique many-body ground states for such a system.

increases with lattice depth! Figure shows this ratio as a function of lattice depth for various double-well barrier heights.

We can show that tunneling of atoms between the MPE states is largely confined to the corresponding ground states. However, these tunneling energies do not have the "correct" bosonic enhancement factors. The system can actually be described by a total effective Hamiltonian of the form,

$$H_{\text{eff}}^{\text{tot}} = \sum_{i} \left\{ \sum_{m=1}^{3} \frac{b_{i}^{\dagger m} b_{i}^{m}}{m!} \Gamma_{m} - J b_{i}^{\dagger} b_{i+1} - \tilde{J} b_{i}^{\dagger} b_{i}^{\dagger} b_{i} b_{i+1} + h.c. \right\}.$$