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

Saurabh Paul, Eite Tiesinga
QuICS, National institute of Standards and Technology
and University of Maryland, College Park, MD, USA

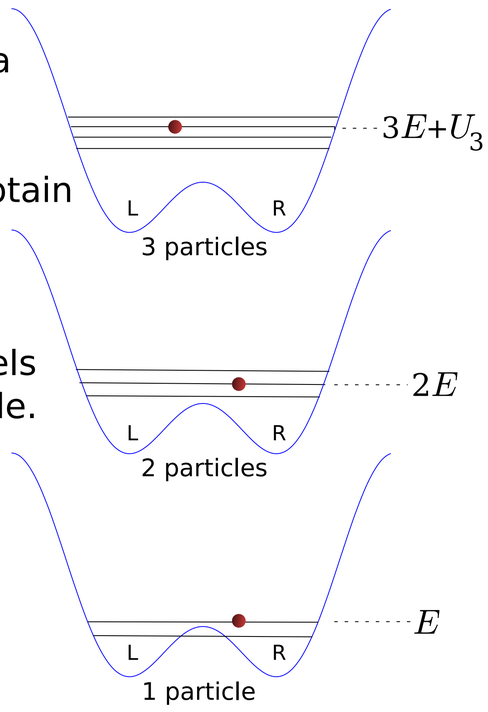
NIST National Institute of Standards and Technology
Technology Administration
U.S. Department of Commerce

1 Introduction

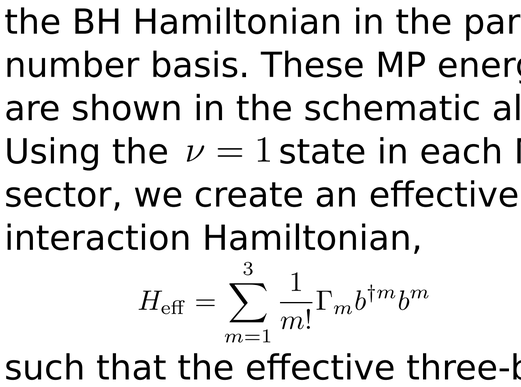
We study ultracold atoms in a double-well optical lattice, with a view to creating an effective Hamiltonian that has large three-body interaction energy. The Bose-Hubbard (BH) Hamiltonian for such a system spans the lowest two bands along x-axis, and the ground band along the perpendicular axes. We obtain the many-particle (MP) states, $|\nu, N\rangle, \nu \in \{1, N+1\}$, 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 sector, we create an effective interaction Hamiltonian,

$$H_{\rm eff} = \sum_{m=1}^{3} \frac{1}{m!} \Gamma_m b^{\dagger m} b^m$$

such that the effective three-body interaction energy is comparable to or larger than the two body term, i.e., $\Gamma_3 \gtrapprox \Gamma_2$. The ratio Γ_3/Γ_2 can be tuned by changing the lattice parameters.



2 Double-well optical lattice and multi-band Hamiltonian



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

The lattice has symmetric double-wells along the x axis, with lattice constant $a = \pi/k_L$, and single wells along the y & z axes. Symmetric double-wells are formed at $k_L b = \pi/4$. A contour plot of the potential in the xy plane is shown in above Figure (left).

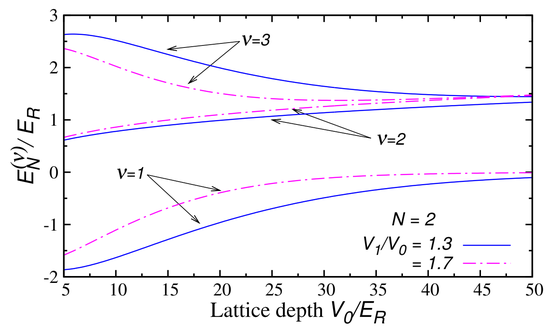
The starting point is the multi-band Hamiltonian, which somewhat simplifies in the band basis, and along x axis is,

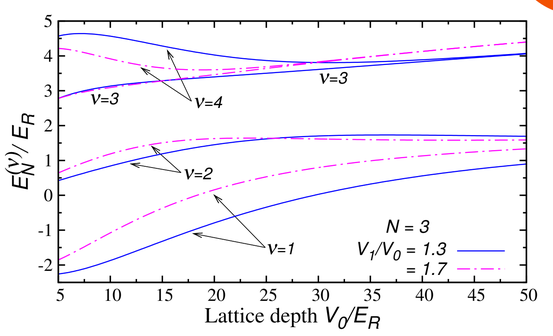
$$H = \sum_i \left\{ \frac{\delta}{2}\left(a^\dagger_{i,2}a_{i,2} - a^\dagger_{i,1}a_{i,1}\right) + \frac{1}{2}\left(U_1 a^\dagger_{i,1}a^\dagger_{i,1}a_{i,1}a_{i,1} + U_2 a^\dagger_{i,2}a^\dagger_{i,2}a_{i,2}a_{i,2}\right) + \frac{1}{2}U_{12}\left(4a^\dagger_{i,1}a_{i,1}a^\dagger_{i,2}a_{i,2} + a^\dagger_{i,1}a^\dagger_{i,1}a_{i,2}a_{i,2} + a^\dagger_{i,2}a^\dagger_{i,2}a_{i,1}a_{i,1}\right) - \sum_{\alpha\in 1,2} J_\alpha\left(a^\dagger_{i,\alpha}a_{i+1,\alpha} + h.c.\right)\right\}$$

where, δ is the band gap between the two lowest bands. All the two-body interaction terms and tunneling energies are obtained numerically from an exact band structure calculation. They are plotted in the above Figure (right). The inset of the Figure shows the numerically obtained Wannier functions for the lowest two energy bands.

The Hamiltonian has a strong pair-tunneling term. The interplay between this term and the band gap plays an important role in determining the behavior of the system.

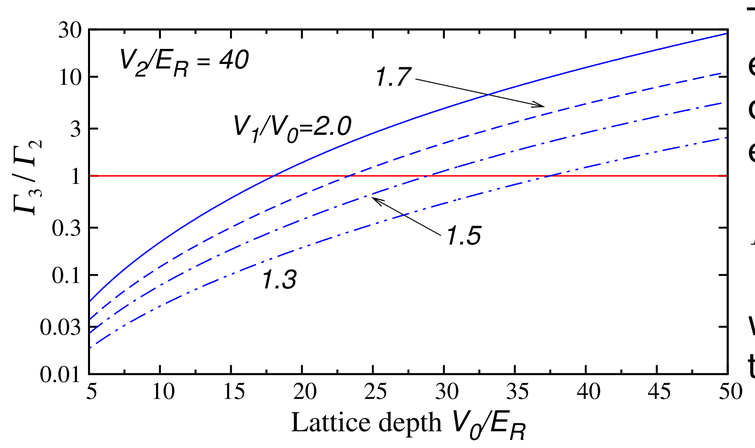
3 Many particle energy (MPE) levels





The interaction part of the Hamiltonian H can be diagonalized in a particle number basis $|n, N\rangle$, where n is the number of atoms in the ground band, while N is the total number of atoms in an unit cell. This gives the MPE 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.

4 Effective three-body interaction



The ground-state MP energies from section 3 can be mapped to an effective Hamiltonian,

$$H^{\rm int}_{\rm eff} = \sum_i \sum_{m=1}^{3} \frac{1}{m!}\Gamma_m b_i^{\dagger m} b_i^m,$$

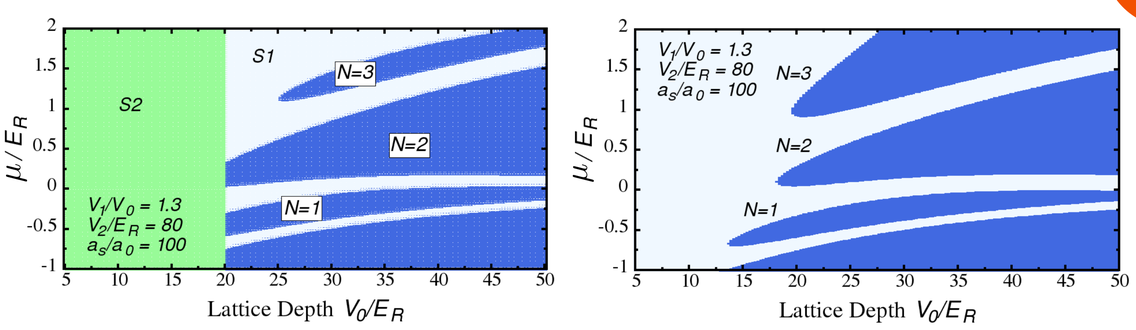
where, Γ_m represents the m-body interaction.

The effective interactions can be expressed in terms of 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, the atoms primarily occupy the ground MP states, and we can show that, $\Gamma_2 \approx \delta$ and $\Gamma_3 \approx 2U_1 \approx 2U_2$. Thus, the ratio Γ_3/Γ_2 increases with lattice depth! Above 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 also largely confined to ground MP states. Interestingly, these tunneling energies between nearest neighbors have the same structure as that for a particle hopping in a single-band Bose-Hubbard model. Thus, the total effective Hamiltonian is,

$$H_{\rm eff} = \sum_i \left\{ \sum_{m=1}^{3} \frac{1}{m!}\Gamma_m b_i^{\dagger m} b_i^m - J_1 b_i^\dagger b_{i+1} + h.c. \right\}.$$

5 Validity of the effective Hamiltonian



The figures show the numerically obtained mean-field phase diagrams for the full and effective Hamiltonians. For $V_0/E_R > 20$, the Mott lobes for $N = 0, 1$ and 2 obtained from both H and $H_{\rm eff}$ are nearly identical. The $N = 3$ lobe, however, is larger for $H_{\rm eff}$. We have to include Γ_4 to correctly model this lobe.

A mean-field calculation using $H_{\rm eff}$ has a single order parameter and does not describe SF phase S2 for $V_0/E_R < 20$.

Summary

We have created an effective Hamiltonian picture to describe a system of ultracold atoms in a double-well potential. This effective Hamiltonian has a large three-body interaction energy, which can be tuned by changing the lattice parameters. In addition, the effective Hamiltonian has nearest-neighbor tunneling energy terms similar in structure to single-band BH model. A comparison between the numerically obtained phase diagrams show remarkable agreement between the full and effective Hamiltonians.

[1] *S. Paul and E. Tiesinga, Physical Review A 92, 023602 (2015)*