Ultracold quantum gases
Problem set no 10

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This weeks exercise deals again with atoms in double wells and optical lattices, but uses numerical techniques:
We will cast the Hamiltonian into a form that can be solved numerically by diagonalizing a matrix. You can do the numerical part in any program you like, e.g. Octave, MATLAB, NumPy or Mathematica (Which is installed in the CIP pool).

1 Double Well with interactions

In this part we consider once more a double well potential with two relevant single-particle Eigenstates, ψ_L and ψ_R in the left resp. right well of the potential. As in the last exercise, we assume that the interactions do not change the form of the wave function within the well. The Hamiltonian of this double well system is given by:

$$\hat{H} = -J\left(\hat{a}_L^\dagger \hat{a}_R + \hat{a}_R^\dagger \hat{a}_L\right) + U \sum_{i\in\{L,R\}} \hat{n}_i\left(\hat{n}_i - 1\right)$$

Here J denotes the strength of the tunnel coupling between the wells and U is a measure of the interaction strength, while $\hat{a}_i^\dagger$ ($\hat{a}_i$) are the usual creation (annihilation) operators for a bosonic particle on site i:

$$\hat{a}_i^\dagger \;|n\rangle_i = \sqrt{n+1}\;|n+1\rangle_i$$
$$\hat{a}_i \;|n\rangle_i = \sqrt{n}\;|n-1\rangle_i$$

Considering a total atom number N,we can write the Fock state with n atoms in the left well and $N-n$ atoms in the right well as:

$$|N,n\rangle = \frac{1}{\sqrt{n!\,(N-n)!}}\left(\hat{a}_L^\dagger\right)^n \left(\hat{a}_R^\dagger\right)^{N-n}\;|0\rangle$$

As these states form a basis of the whole Hilbert space, every state $|\Psi\rangle$ can be written as a superposition of these basis states: $|\Psi\rangle = \sum_k c_k\, |N,k\rangle$ with the c_k denoting complex numbers. In this way we can represent every state by a vector C consisting of the coefficients c_k and the time-independent Schrdinger equation $\hat{H}\, |\Psi\rangle = E\, |\Psi\rangle$ can be written as an Eigenvector equation:

$$\begin{pmatrix} H_{1,1} & H_{1,2} & \cdots & H_{1,N+1} \\ H_{2,1} & H_{2,2} & \cdots & H_{2,N+1} \\ \cdots & \cdots & \cdots & \cdots \\ H_{N+1,1} & H_{N+1,2} & \cdots & H_{N+1,N+1} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \cdots \\ c_{N+1} \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \\ \cdots \\ c_{N+1} \end{pmatrix}$$

- Calculate the matrix elements $H_{i,j} = \langle N, i-1|\, \hat{H}\, |N, j-1\rangle$ of the Hamiltonian. You should get:

$$\begin{aligned} H_{i,j} = & -J\left(\sqrt{j}\sqrt{N-j+1}\,\delta_{i-1,j} + \sqrt{j-1}\sqrt{N-j+3}\,\delta_{i+1,j}\right) \\ & + U\left\{(i-1)(i-2) + (N-i+1)(N-i)\right\}\delta_{i,j} \end{aligned}$$

- Diagonalize the resulting Hamiltonian (the resulting matrix) in the case of $J = 1$ and $U = 0$ for several N and compare the resulting number distribution on a given site with a binomial distribution. (Hint: All of the above mentioned programs have build-in functions to perform the diagonalization!)
- Now diagonalize the Hamiltonian for finite interactions and describe the change in the number distributions.
- What is the difference between even and odd total atom numbers, and how can it be explained intuitively?

2 Single atom on a 1D lattice

Now consider a single atom in the lowest band of a 1D lattice with N_l lattice sites and nearest neighbor tunneling J. Neglect any constant on-site terms.

- Write the Hamiltonian as a matrix in the Wannier basis and diagonalize it.
- Plot the ground state energy as a function of the number of lattice sites. Does it approach any limiting value?
- optional: Calculate the quasi-momentum distribution by performing a discrete Fourier transformation of the coefficients c_k. (This is equivalent to expressing the Bloch waves as a superposition of Wannier states.)

3 Many-atoms in many-wells

Unfortunately it is impossible to use the above methods (that are called exact diagonalization techniques) in the most interesting case of many interacting atoms in a lattice. In order to see this, calculate the number of basis states for N_A identical bosons in a lattice with N_l lattice sites.