Lesson 10 - Bosons in a double-well potential
Unit 10.1 Bose-Hubbard Hamiltonian

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Dimensional reduction (I)

The starting point is the quantum-field-theory Hamiltonian

$$\hat{H} = \int d^3\mathbf{r} \; \hat{\psi}^+(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \frac{1}{2}\int d^3\mathbf{r} \; d^3\mathbf{r}' \; \hat{\psi}^+(\mathbf{r}) \; \hat{\psi}^+(\mathbf{r}') \; V(\mathbf{r}-\mathbf{r}') \; \hat{\psi}(\mathbf{r}') \; \hat{\psi}(\mathbf{r}), \quad (1)$$

where the external trapping potential is given by

$$U(\mathbf{r}) = V_{DW}(x) + \frac{1}{2} m\omega_\perp^2 (y^2 + z^2) \; , \quad (2)$$

that is a generic double-well potential $V_{DW}(x)$ in the x axial direction and a harmonic potential in the transverse (y, z) plane.
We assume that the system of bosons, described by the field operator $\hat{\psi}(\mathbf{r})$, is dilute and approximate the inter-particle potential with a contact Fermi pseudo-potential, namely

$$V(\mathbf{r}-\mathbf{r}') = g\,\delta(\mathbf{r}-\mathbf{r}') \; , \quad (3)$$

with g the strength of the interaction.

Dimensional reduction (II)

If the frequency $\omega_\perp$ of transverse confinement is sufficiently large, the system is quasi-1D and the bosonic field operator can be written as

$$\hat{\psi}(\mathbf{r}) = \hat{\phi}(x) \, \frac{e^{-(y^2+z^2)/(2l_\perp^2)}}{\pi^{1/2} l_\perp} \; . \tag{4}$$

We are thus supposing that in the transverse (y, z) plane the system is Bose-Einstein condensed into the transverse single-particle ground-state, which is a Gaussian wavefunction of width

$$l_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}} \; , \tag{5}$$

that is the characteristic length of the harmonic confinement.

Dimensional reduction (III)

Inserting Eq. (4) into the Hamiltonian (1) and integrating over y and z variabiles we obtain the effective 1D Hamiltonian

$$\begin{aligned}\hat{H} &= \int dx\ \hat{\phi}^{+}(x)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_{DW}(x) + \hbar\omega_{\perp}\right]\hat{\phi}(x) \\ &+ \frac{g_{1D}}{2}\int dx\ \hat{\phi}^{+}(x)\ \hat{\phi}^{+}(x)\ \hat{\phi}(x)\ \hat{\phi}(x)\ ,\end{aligned} \tag{6}$$

where

$$g_{1D} = \frac{g}{2\pi l_{\perp}^2} \tag{7}$$

is the effective 1D interaction strength.

Double-well potential and two-mode approximation (I)

We suppose that the barrier of the double-well potential $V_{DW}(x)$, with its maximum located at $x = 0$, is quite high such that there several doublets of quasi-degenerate single-particle energy levels.

Moreover, we suppose that only the lowest doublet (i.e. the single-particle ground-state and the single-particle first excited state) is occupied by bosons. Under these assumptions we can write the bosonic field operator as

$$\hat{\phi}(x) = \hat{a}_L \, \phi_L(x) + \hat{a}_R \, \phi_R(x) \tag{8}$$

that is the so-called two-mode approximation, where $\phi_L(x)$ and $\phi_R(x)$ are single-particle wavefunctions localized respectively on the left well and on the right well of the double-well potential.

These wavefunctions (which can be taken real) are linear combinations of the even wavefunction $\phi_0(x)$ of the ground state and the odd wavefunction $\phi_1(x)$ of the first excited state.
Clearly the operator $\hat{a}_j$ annihilates a boson in the j-th site (well) while the operator $\hat{a}_j^+$ creates a boson in the j-th site $(j = L, R)$

Bose-Hubbard Hamiltonian (I)

Inserting the two-mode approximation (8) of the bosonic field operator in the effective 1D Hamiltonian, we get the following two-site Hamiltonian

$$\hat{H} = \epsilon_L \hat{N}_L + \epsilon_R \hat{N}_R - J_{LR} \hat{a}_L^+ \hat{a}_R - J_{RL} \hat{a}_R^+ \hat{a}_L + \frac{U_L}{2} \hat{N}_L (\hat{N}_L - 1) + \frac{U_R}{2} \hat{N}_R (\hat{N}_R - 1) , \quad (9)$$

where $\hat{N}_j = \hat{a}_j^+ \hat{a}_j$ is the number operator of the j-th site,

$$\epsilon_j = \int dx \; \phi_j(x) \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_{DW}(x) + \hbar\omega_\perp \right] \phi_j(x) \quad (10)$$

is the kinetic plus potential energy on the site j,

$$J_{ij} = \int dx \; \phi_i(x) \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_{DW}(x) + \hbar\omega_\perp \right] \phi_j(x) \; , \quad (11)$$

is the hopping energy (tunneling energy) between the site i and the site j, and

$$U_j = g_{1D} \int dx \; \phi_j(x)^4 \quad (12)$$

is the interaction energy on the site j.

Bose-Hubbard Hamiltonian (II)

The Hamiltonian (9) is the two-site Bose-Hubbard Hamiltonian, named after John Hubbard introduced a similar model in 1963 to describe fermions (electrons) on a periodic lattice.
If the double-well potential $V_{DW}(x)$ is fully symmetric then $\epsilon_L = \epsilon_R = \epsilon$, $J_{LR} = J_{RL} = J$, $U_L = U_R = U$, and the Bose-Hubbard Hamiltonian becomes

$$\hat{H} = \epsilon \left(\hat{N}_L + \hat{N}_R \right) - J \left(\hat{a}_L^+ \hat{a}_R + \hat{a}_R^+ \hat{a}_L \right) + \frac{U}{2} \left[\hat{N}_L(\hat{N}_L - 1) + \hat{N}_R(\hat{N}_R - 1) \right] . \tag{13}$$

The two-site Bose-Hubbard Hamiltonian can be easily extendend to L sites as follows

$$\hat{H} = \epsilon \sum_{j=1}^{L} \hat{N}_j - J \sum_{j=1}^{L-1} \left(\hat{a}_j^+ \hat{a}_{j+1} + \hat{a}_{j+1}^+ \hat{a}_j \right) + \frac{U}{2} \sum_{j=1}^{L} \hat{N}_j(\hat{N}_j - 1) . \tag{14}$$

Actually the first term, which contains the total number of particles $\hat{N} = \sum_{j=1}^{L} \hat{N}_j$, does not affect the dynamical properties of the system.