Exercise 1: The coherent state

Show that the expression of the coherent state $|\alpha\rangle$ (recall the exercise in the Präsenzbungen) in terms of the number state $|n\rangle$ is given by

$$|\alpha\rangle = \mathrm{e}^{-|\alpha|^2/2} \sum_{\mathrm{n}=0}^{\infty} \frac{\alpha^{\mathrm{n}}}{\sqrt{\mathrm{n}!}} |\mathrm{n}\rangle. \tag{1}$$

Exercise 2: Number operator and Hamiltonian

Show, for bosons and fermions, that the particle-number operator $\hat{N} = \sum_i \hat{a}_i^\dagger \hat{a}_i$ commutes with the Hamiltonian

$$\hat{H} = \sum_{i,j} \hat{a}_i^\dagger \langle i|\hat{T}|j\rangle \hat{a}_j + \frac{1}{2} \sum_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \langle ij|\hat{V}|kl\rangle \hat{a}_l \hat{a}_k. \tag{2}$$

What is the physical meaning of $\left[\hat{N}, \hat{H}\right] = 0$?

Exercise 3: The Hubbard model

Consider electrons on a lattice with the single-particle wave function localized at the lattice point $\mathbf{R}_i$ given by $\varphi_{i\sigma}(\mathbf{x}) = \chi_\sigma \varphi_i(\mathbf{x})$ with $\varphi_i(\mathbf{x}) = \phi(\mathbf{x} - \mathbf{R}_i)$. A Hamiltonian, $\hat{H} = \hat{T} + \hat{V}$, consisting of a spin-independent single-particle operator $\hat{T} = \sum_{\alpha=1}^{N} t_\alpha$ and a two-particle operator $\hat{V} = \frac{1}{2} \sum_{\alpha \neq \beta} V^{(2)}(\mathbf{x}_\alpha, \mathbf{x}_\beta)$ can be represented in the basis $\{\varphi_{i\sigma}\}$ by

$$\hat{H} = \sum_{i,j} \sum_{\sigma} t_{ij} \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} + \frac{1}{2} \sum_{i,j,k,l} \sum_{\sigma,\sigma'} V_{ijkl} \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma'}^\dagger \hat{a}_{l\sigma'} \hat{a}_{k\sigma}, \tag{3}$$

where the matrix elements are given by $t_{ij} = \langle i|t|j\rangle$ and $V_{ijkl} = \langle ij|V^{(2)}|kl\rangle$. If one assumes that the overlap of the wave functions $\varphi_i(\mathbf{x})$ at different lattice points is negligible, one can make the following approximations:

$$t_{ij} = \begin{cases} w & \text{for } i = j, \\ t & \text{for i and j adjacent sites,} \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

$$V_{ijkl} = V_{ij} \delta_{il} \delta_{jk} \quad \text{with } V_{ij} = \int \mathrm{d}^3x \int \mathrm{d}^3y |\varphi_i(\mathbf{x})|^2 V^{(2)}(\mathbf{x}, \mathbf{y}) |\varphi_j(\mathbf{y})|^2. \tag{5}$$

(a) Determine the matrix elements V_{ij} for a contact potential

$$V = \frac{\lambda}{2} \sum_{\alpha \neq \beta} \delta(\mathrm{x}_\alpha - \mathrm{x}_\beta) \tag{6}$$

between the electrons for the following cases: (i) on-site interaction $i = j$, and (ii) nearest-neighbor interaction, i.e., i and j adjacent lattice points. Assume a square lattice with lattice constant a and wave functions that are Gaussians $\varphi(\mathrm{x}) = \frac{1}{\Delta^{3/2}\pi^{3/4}} \exp\{-\mathrm{x}^2/2\Delta^2\}$.

(b) In the limit $\Delta \ll a$, the on-site interaction $U = V_{ii}$ is the dominant contribution. Determine for this limiting case the form of the Hamiltonian in second quantization. The model thereby obtained is known as the *Hubbard model.*

Exercise 4: The Bose-Hubbard model

Consider the Hubbard model for bosons

$$\hat{H} = -t \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_{i=1}^{N_{site}} \hat{n}_i(\hat{n}_i - 1). \tag{7}$$

(a) Show that the $N-$particle state

$$|\Psi_{U=0}\rangle = \frac{1}{\sqrt{N}} \left(\frac{1}{\sqrt{N_{site}}} \sum_{i=1}^{N_{site}} \hat{a}_i^\dagger \right)^N |0\rangle \tag{8}$$

for $U = 0$ is an eigenstate of $\hat{H}$. How is the energy of this state? What is the physical meaning of $\frac{1}{\sqrt{N_{site}}} \sum_{i=1}^{N_{site}} \hat{a}_i^\dagger$?(Hint: Think in momentum space.)

(b) Show that the state

$$|\Psi_{t=0}\rangle = \prod_{i=1}^{N_{site}} \hat{a}_i^\dagger |0\rangle \tag{9}$$

for $t = 0$ is an eigenstate of $\hat{H}$. How is the energy of this state?