PHY635, I-Semester 2019/20, Assignment 1

Instructor: Sebastian Wüster
Due-date: Lecture 16.8.2019

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(1) Many body wave functions: Translate the following sentences into math, i.e. write down the described quantum many-body states. For each first assume the particles are distinguishable, then also specify the wave function for indistinguishable Bosons or Fermions. In each case, make a 2D contour drawing of the wave-functions. [8 points]:

(i) One is in the ground-state of the harmonic oscillator, and another has momentum $p_0 > 0$.

(ii) Two particles of mass M are bound to each other, with a wave-function the modulus of which drops of as $\exp\left[-r/\xi\right]$ with separation r between them. The compound object created has momentum p_0.

(iii) Particle one is localized with Gaussian shape and width σ_1 near x_a. Particle two near x_b with width σ_2.

(iv) The same as in (iii), for $x_a = x_b = 0$ and $\sigma_1 = \sigma_2 = \sigma$, but due to some interactions, the particles avoid each other, such that the probability to find them a distance r apart drops of as $p(r) \sim \tanh(r/\xi)^2$, with $\xi \ll \sigma_{1,2}$

(2) Ladder operators: Determine the following matrix elements for Bosonic operators/states in a three mode problem [6 points]

$$\begin{aligned}
\mathcal{M}_1 &= \langle\, 110\,|\hat{a}_2\hat{a}_2^\dagger\hat{a}_2^\dagger|\,101\,\rangle, & \mathcal{M}_2 &= \langle\, 110\,|\hat{a}_2^\dagger\hat{a}_2^\dagger\hat{a}_2|\,101\,\rangle,\\
\mathcal{M}_3 &= \langle\, 113\,|\hat{a}_3^\dagger|\,112\,\rangle, & \mathcal{M}_4 &= \langle\, 223\,|\hat{a}_2^\dagger|\,113\,\rangle,\\
\mathcal{M}_5 &= \langle\, 010\,|\hat{a}_2^\dagger\hat{a}_3|\,001\,\rangle, & \mathcal{M}_6 &= \langle\, 302\,|\hat{a}_2\hat{a}_3^\dagger|\,301\,\rangle.
\end{aligned} \tag{1}$$

Determine the following matrix elements for Fermionic operators/states in a three mode problem [6 points]

$$\begin{aligned}
\mathcal{M}_1 &= \langle\, 110\,|\hat{a}_2\hat{a}_2^\dagger\hat{a}_2^\dagger|\,101\,\rangle, & \mathcal{M}_2 &= \langle\, 110\,|\hat{a}_2\hat{a}_2^\dagger\hat{a}_2^\dagger\hat{a}_2|\,110\,\rangle,\\
\mathcal{M}_3 &= \langle\, 110\,|\hat{a}_1^\dagger\hat{a}_1\hat{a}_3\hat{a}_3^\dagger|\,110\,\rangle, & \mathcal{M}_4 &= \langle\, 001\,|\hat{a}_2^\dagger|\,010\,\rangle,\\
\mathcal{M}_5 &= \langle\, 010\,|\hat{a}_2^\dagger\hat{a}_3|\,001\,\rangle, & \mathcal{M}_6 &= \langle\, 101\,|\hat{a}_2\hat{a}_3^\dagger|\,001\,\rangle.
\end{aligned} \tag{2}$$

(3) Hamiltonian in second quantisation: Consider a multi-electron atom such as Uranium, let us say N_e electrons. The Hamiltonian in atomic units is

$$\hat{H} = \sum_{i=1}^{N_e} \left(-\frac{1}{2}\nabla^2_{\mathbf{r}_i} - \frac{Z}{r_i} \right) + \sum_{i<j=1}^{N} \frac{1}{r_{ij}}, \tag{3}$$

where $\mathbf{r}_j$ is the position of electron j relative to the nucleus, $r_j = |\mathbf{r}_j|$ and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ and Z the nuclear charge. Use the single particle basis of spin-less Hydrogenic states $|\,\varphi_{nlm}\,\rangle$ fulfilling $\hat{H}_Z|\,\varphi_{nlm}\,\rangle = E_n|\,\varphi_{nlm}\,\rangle$ with $\hat{H}_Z = -\frac{1}{2}\nabla^2_{\mathbf{r}} - \frac{Z}{r}$ and associated Fermionic creation operators $\hat{a}_{nlm}$, to convert that Hamiltonian into a second quantized form [10 points].

(4) Numerical Quantum Many Body Physics Consider two coupled quantum mechanical harmonic oscillators of mass $m = 1$ and frequency $\omega = 1$, described with the first quantized Hamiltonian

$$H = \frac{1}{2}\left(p_1^2 + x_1^2\right) + \frac{1}{2}\left(p_2^2 + x_2^2\right) + 2\kappa x_1 x_2, \tag{4}$$

where x_i is the position of oscillator i and p_i its momentum.

(4a) Write down the corresponding two-body Schrödinger equation for a wave function $\Psi(x_1, x_2)$ in the position space representation. You may treat the oscillators as distinguishable. [3 points]

(4b) In terms of $\Psi(x_1, x_2)$, also derive expressions for the energy expectation value, and split it into energy of oscillator 1, energy of oscillator 2 and interaction energy. [2 points]

(4c) Edit the template file `Assignment1_phy635_program_draft_v1.xmds` provided online. It presently contains the Schrödinger equation and energy sampling as appropriate when particle 1 is a free particle and particle 2 is ignored. Edit this to include your results from (4a), (4b). [1 points]

(4d) Implement as initial condition for the wave function $\Psi(x_1, x_2) = \frac{1}{\sqrt{\sqrt{\pi}\sigma}} \exp\left(-\frac{x_1^2}{2\sigma^2}\right) \frac{x_2\sqrt{2}}{\sigma\sqrt{\sqrt{\pi}\sigma}} \exp\left(-\frac{x_2^2}{2\sigma^2}\right)$, and convince yourself that this corresponds to oscillator 1 in the ground state and oscillator 2 in the excited state. Follow the info-sheet `Numerics_assignments_info.pdf` to run your code until time $t_{fin} = 100$ once implemented. First, check that normalisation and total energy are conserved, using `Assignment1_plot_checks_v1.m`. Then check the individual energy components using `Assignment1_plot_energies_v1.m`. Discuss your results. Also inspect the actual evolution of the many-body density using `Assignment1_density_slideshow_v1.m`, and comment on that as well. [4 points]