PHY635, II-Semester 2022/23, Assignment 1

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Due-date: Email to TA by 13.1.2023

(1) Two-body wave functions: Consider two particles in one dimension, one at position r_1 and the other at r_2. Translate the following sentences into math, i.e. write down the described quantum many-body states. For each first assume the two particles are distinguishable, then also specify the wave function for indistinguishable Bosons or Fermions. In each case, make a 2D contour drawing in the space (r_1, r_2) of the wave-functions, indicating signs or Re and Im as well. [6 points]:

(a) One is in the $n = 1$ state of the harmonic oscillator, and the other in $n = 2$.

(b) Neutron A is stuck in a nucleus between $r_1 = 0$ and $r_2 = R$ in its ground-state, while neutron B impinges on the nucleus from negative r_2 and elastically scatters off it in the backwards direction.

(c) Particle A is localized with Gaussian wavefunction and width σ_A near x_A. Particle B near x_B with width σ_B. Compare the two cases (i) $\sigma_A = \sigma_B = \sigma \ll |x_A - x_B|$ and (ii) $\sigma_A = \sigma_B = \sigma \approx |x_A - x_B|$, separately for indistinguishable particles, Bosons and Fermions.

(2) Creation and destruction operators:

(a) Let $\hat{a}_k$ be a *fermionic* destruction operator for a multi-mode system, with index k numbering the mode. Find the simplest expression for the operator product

$$\hat{a}_k^\dagger \hat{a}_\ell \hat{a}_\ell^\dagger \hat{a}_k^\dagger \hat{a}_k \tag{1}$$

and justify your answer [2ps].

(b) Consider a bosonic two-mode problem, with $\hat{a}$, $\hat{b}$ the destruction operator for the two modes, and $|\, n, m\,\rangle$ the Fock states describing them. We define the operators $\hat{C} = \hat{a}^\dagger \hat{a} + \hat{b}^\dagger \hat{b}$, $\hat{D} = \hat{a}^\dagger \hat{a} - \hat{b}^\dagger \hat{b}$. First give a physical interpretation of both. Then write the most general separable two-mode state, compare the variance of $\hat{C}$ and $\hat{D}$ and discuss [2pts].

(3) Hamiltonian in second quantisation: Consider N_e electrons in some external potential $V(\mathbf{x})$, for example the lattice potential of the ion crystal in a a solid material, interacting through Coulomb interactions with Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N_e} \left(-\frac{\hbar^2}{2m_e} \nabla^2_{\mathbf{r}_i} + V(\mathbf{r}_i) \right) + \sum_{i<j=1}^{N} \frac{e^2}{(4\pi\epsilon_0)|\mathbf{r}_i - \mathbf{r}_j|}, \tag{2}$$

where $\mathbf{r}_j$ is the position of electron j. Use the single particle basis $|\,\sigma, \mathbf{k}\,\rangle$, corresponding to an electron with spin (z-component) $\sigma \in \{\uparrow, \downarrow\}$ and wavenumber $\mathbf{k}$ to convert Eq. (2) into a second quantised Hamiltonian, for operators $\hat{a}_{\sigma\mathbf{k}}$ ($\hat{a}^\dagger_{\sigma\mathbf{k}}$). Use box-quantised plane wave states, i.e. $\langle\, \mathbf{x}\,|\,\sigma, \mathbf{k}\,\rangle = \frac{1}{\mathcal{V}} e^{i\mathbf{k}\cdot\mathbf{x}}\xi_\sigma$, where ξ_σ is a spinor. Discuss each term in your Hamiltonian, what is physically implies, why it takes the form it takes, and what conservation laws might be encoded in it. [10 points].

(4) Numerical Quantum Many Body Physics Consider two indistinguishable particles at r_1 and r_2 (either Fermions or Bosons), moving in one dimension and interacting with a Gaussian potential (for simplicity). Their Hamiltonian thus is:

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2}\right) + Ae^{-\frac{(r_1-r_2)^2}{2S^2}} \tag{3}$$

where A is an interaction strength and S an interaction range.

(4a) Find the two-body Schrödinger equation, then express everything in terms of a centre of mass (CM) coordinate $R = (r_1 + r_2)/2$ and a relative coordinate $r = r_2 - r_1$, and show that if two separate Schrödinger equations for the CM and relative motion are fulfilled, the origial equation is fulfilled. For this use the Ansatz $\Psi(r_1, r_2, t) = \phi(r, t)\varphi(R, t)$ for the two-body wavefunction. Discuss how the centre of mass wavefunction $\varphi(R, t)$ evolves. [2 points]

(4b) Discuss which symmetry properties the relative wavefunction $\phi(r)$ must have for indistinguishable Bosons and Fermions. How does that differ from the properties of the wavefunction for distinguishable particles? [2 points]

(4c) The code `Assignment1_phy635_program_draft_v1.xmds` is setup to model scattering of the two particles discussed above for potential with $A = A_1 = 3$ and $S = 2$, initially treating the particles as (i) distinguishable with initial wavefunction $\phi(r, t = 0) = \mathcal{N}e^{-\frac{(r-r_0)^2}{2\sigma^2}}e^{-ikr}$ (do not change parameters of that wavepacket). Edit the code such that it can also treat the particles as (ii) Bosons and (iii) Fermions. For each of (i)-(iii) run it for the parameters above, as well as $A = A_2 = 0.8$. Use the script `Assignment1_plot_reldens_v1.m` to plot the probability density of the relative coordinate r for all six cases. [3 points]

(4d) Discuss and compare your six different results from (b) in the context of the cartoon shown in the lecture on page 12 (above Eq. (1.33)) [3 points]