CEM 991 **Fall 2021**

Assignment No. 3 (25 pts.) **Due Date: October 15, 2021 (Friday)**

1. (6 pts.) The $1s$ and $2s$ states of the hydrogen atom are described by the wave functions

$$u_{1s}(r) = \frac{1}{\sqrt{\pi}} a_0^{-\frac{3}{2}} e^{-\frac{r}{a_0}}, \tag{1}$$

$$u_{2s}(r) = \frac{1}{\sqrt{32\pi}} a_0^{-\frac{3}{2}} (2 - \frac{r}{a_0}) e^{-\frac{r}{2a_0}}, \tag{2}$$

where r is the distance from the origin and a_0 is the radius of the first circular Bohr orbit.

   (a) Show that u_{1s} and u_{2s} are normalized to unity.

   (b) Compute the expectation value of r in the state described by u_{1s}.

   Auxiliary formula: $\int_0^\infty x^n e^{-\alpha x} dx = \frac{n!}{\alpha^{n+1}}$, $\alpha > 0$, $n = 0, 1, 2, \dots$.

2. (4 pts.) The wave function of a freely moving particle in one dimension has the form,

$$\psi(x) = A e^{ikx}, \tag{3}$$

where A is a constant and $p = k\hbar$ is the momentum of a particle. Calculate the probability current density for this particle and compare the result with the equation from hydrodynamics,

$$\mathbf{j} = \rho \mathbf{v}, \tag{4}$$

where $\mathbf{j}$ and ρ are current density and density of the fluid, respectively, and $\mathbf{v}$ is the fluid velocity.$^{\#)}$

3. (7 pts.) Consider a three-dimensional wave packet $\psi = \psi(x, y, z, t)$ under the influence of a force derived from the real potential $V = V(x, y, z, t)$. The mass of the corresponding classical particle is designated by m. Show that

$$\frac{d}{dt}\langle \hat{L}_z \rangle = \langle \hat{D}_z \rangle, \tag{5}$$

where, in general,

$$\langle \hat{F} \rangle = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \psi^* \hat{F} \psi \, dx dy dz \tag{6}$$

represents the expectation value of the operator $\hat{F}$, $\hat{L}_z$ is the z component of the angular momentum operator, and

$$\hat{D}_z = \left(-\hat{x} \frac{\partial \hat{V}}{\partial y} \right) - \left(-\hat{y} \frac{\partial \hat{V}}{\partial x} \right). \tag{7}$$

Please comment on the result.
Hint: Use the fact that ψ represents a solution of the Schrödinger equation,

$$\imath\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi, \tag{8}$$

and the property of the Laplacian,

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\psi^*(\nabla^2\phi)dxdydz = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}(\nabla^2\psi)^*\phi dxdydz, \tag{9}$$

or the fact that the kinetic energy operator is Hermitian.

4. (8 pts.) Calculate the following commutators:

   (a) $[\hat{x}, \hat{p}_x^2]$,

   (b) $[\hat{x}^2, \hat{p}_x]$,

   (c) $[\hat{x}^2, \hat{p}_x^2]$

   ($\hat{p}_x$ is the x-component of the momentum operator $\hat{\mathbf{p}}$). Use (a)–(c) to evaluate the commutator $[\hat{x}, \hat{H}]$, where $H = \frac{p_x^2}{2m} + V(x)$ is the Hamiltonian.
   Hint: In evaluating the commutators (a)–(c), use the formula $[\hat{x}, \hat{p}_x] = \imath\hbar\mathbf{1}$, where $\mathbf{1}$ is the unit operator, and exploit properties of a commutator, such as $[\hat{F}_1\hat{F}_2, \hat{G}] = \hat{F}_1[\hat{F}_2, \hat{G}] + [\hat{F}_1, \hat{G}]\hat{F}_2$ (cf. Problem 5 of Assignment No. 2). In other words, use an algebraic approach.

#) Bold symbols designate vector quantities.