

# Homework 3

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## 1

### 1.1

In order to keep the matrix elements invariant, in the Heisenberg picture we have

$$O_H = e^{iHt/\hbar} O_S e^{-iHt/\hbar}, \quad (1)$$

so that

$${}_H \langle \psi' | O_H | \psi \rangle_H = {}_S \langle \psi' | O_S | \psi \rangle_S. \quad (2)$$

The differential time evolution equation is

$$\frac{dO_H}{dt} = \frac{i}{\hbar} H O_H - O_H \cdot \frac{i}{\hbar} H + e^{iHt/\hbar} \frac{\partial O_S}{\partial t} e^{-iHt/\hbar}, \quad (3)$$

and therefore

$$\begin{aligned} \frac{d\langle O \rangle}{dt} &= \frac{1}{i\hbar} \langle \psi_H | [O_H, H] | \psi_H \rangle + \langle \psi_H | e^{iHt/\hbar} \frac{\partial O_S}{\partial t} e^{-iHt/\hbar} | \psi_H \rangle \\ &= \frac{1}{i\hbar} \langle \psi_H | [O_H, H] | \psi_H \rangle + \langle \psi_S | \frac{\partial O_S}{\partial t} | \psi_S \rangle \\ &= \frac{1}{i\hbar} \langle [O, H] \rangle + \left\langle \frac{\partial O}{\partial t} \right\rangle. \end{aligned} \quad (4)$$

Note: here we assume  $H$  has no time dependence, and thus the time evolution operator assumes the simple form  $e^{-iHt/\hbar}$ . The condition that  $H$  has no time dependence also means in the Heisenberg picture,  $H_H(t) = H_H(0)$ , and on the other hand,  $H_H(t)$  can be obtained from  $H_H(0)$  by replacing the values of all operators at  $t = 0$  to the corresponding values at  $t$ , and therefore the commutation relation  $[O_H(t), H]$  can be obtained by replacing the occurrences of all operators in  $[O_H(t=0), H] = [O_S, H]$  with their values at  $t$ . That's why in the third line, we omit the Heisenberg/Schrodinger picture labels.

### 1.2

Since the Hamiltonian

$$H = \frac{p^2}{2m} + V \quad (5)$$

is real (and not just Hermitian), we can always obtain real eigenfunctions. Thus

$$\begin{aligned} \int dx \psi^* x (-i\hbar) \partial_x \psi &= -i\hbar \psi^* x \psi \Big|_{x=-\infty}^{\infty} + i\hbar \int dx \partial_x (\psi^* x) \psi \\ &= i\hbar \int dx \partial_x (x\psi) \psi = i\hbar \int dx \psi^2 + i\hbar \int dx x (\partial_x \psi) \psi \\ &= i\hbar \int dx |\psi|^2 - \int dx \psi^* x (-i\hbar \partial_x) \psi, \end{aligned}$$

and therefore

$$\begin{aligned} 2 \int dx \psi^* x p \psi &= i\hbar, \\ \langle xp \rangle &= i\hbar/2. \end{aligned} \quad (6)$$

Therefore

$$0 = \frac{d}{dt} \langle xp \rangle = \frac{1}{i\hbar} \langle [xp, H] \rangle.$$

The commutation relation can be evaluated as (note the correspondence between Poisson brackets and commutators)

$$\begin{aligned} [xp, H] &= \frac{1}{2m} [xp, p^2] + [xp, V(x)] \\ &= \frac{1}{2m} [x, p^2] p + x[p, V(x)] \\ &= \frac{1}{2m} \cdot 2i\hbar p \cdot p - x \cdot i\hbar \frac{\partial V(x)}{\partial x}, \end{aligned}$$

so we find

$$0 = i\hbar \left\langle \frac{p^2}{m} \right\rangle - i\hbar \left\langle x \frac{\partial V(x)}{\partial x} \right\rangle,$$

and therefore

$$2 \langle T \rangle = \left\langle x \frac{\partial V(x)}{\partial x} \right\rangle. \quad (7)$$

### 1.3

The proof can be repeated by replacing  $x(-i\hbar)\partial_x$  by  $\mathbf{x} \cdot (-i\hbar)\nabla$ . We then have

$$\begin{aligned} \int d^3\mathbf{x} \psi^* \mathbf{x} \cdot (-i\hbar)\nabla \psi &= -i\hbar \oint d\mathbf{S} \cdot (\psi^* \mathbf{x} \psi) + i\hbar \int d^3\mathbf{x} \nabla \cdot (\psi^* \mathbf{x} \psi) \\ &= i\hbar \int d^3\mathbf{x} \nabla \cdot (\psi \mathbf{x}) \psi \\ &= i\hbar \int d^3\mathbf{x} \psi^2 \underbrace{\nabla \cdot \mathbf{x}}_3 + i\hbar \int d^3\mathbf{x} \psi \mathbf{x} \cdot \nabla \psi, \end{aligned}$$

and we find

$$2 \langle \mathbf{x} \cdot \mathbf{p} \rangle = 3i\hbar. \quad (8)$$

Then repeating the derivation above, we get

$$2 \langle T \rangle = \left\langle \mathbf{x} \cdot \frac{\partial V(\mathbf{x})}{\partial \mathbf{x}} \right\rangle. \quad (9)$$

### 1.4

When  $V = -1/r$ , we have

$$E = \langle V \rangle + \frac{1}{2} \left\langle r \frac{\partial V}{\partial r} \right\rangle = - \left\langle \frac{1}{r} \right\rangle + \frac{1}{2} \left\langle r \cdot \frac{1}{r^2} \right\rangle = - \frac{1}{2} \left\langle \frac{1}{r} \right\rangle < 0, \quad (10)$$

and therefore bound states are possible. When  $V = -1/r^2$ , however, we have

$$E = \langle V \rangle + \frac{1}{2} \left\langle r \frac{\partial V}{\partial r} \right\rangle = - \left\langle \frac{1}{r^2} \right\rangle + \frac{1}{2} \left\langle r \cdot \frac{2}{r^3} \right\rangle = 0, \quad (11)$$

which causes a contradiction: if a bound state exists, then its energy is not below  $E = 0$ . Thus the potential  $V(r) = -1/r^2$  doesn't assume bound states.

## 2

We want to calculate

$$P_{\text{stay}} = |\langle \text{old ground} | U | \text{new ground} \rangle|^2. \quad (12)$$

If the Hamiltonian of a system undergoes a sudden change at  $t = 0$  and assumes now time evolution beside this point, the time evolution operator  $U(t, 0)$  is trivial both when  $t > 0$  and  $t < 0$ , and the probability is

$$P_{\text{say}} = |\langle \text{old ground} | \text{new ground} \rangle|^2. \quad (13)$$

Now suppose  $\psi_0$  is the 1s orbital of the electron in a hydrogen atom. The hydrogen atom obtains a momentum  $-k\hat{z}$  after scattering with an  $\alpha$  particle. In the frame of reference attached to the hydrogen atom after scattering, the old ground state is moving with momentum  $k\hat{z}$ , and its wave function therefore should be

$$\psi_{k0}(\mathbf{r}) = e^{ikz}\psi_0(\mathbf{r}). \quad (14)$$

The possibility for the electron to stay at the ground state after the collision – in other words, the possibility for the electron to go from the old ground state to the new ground state – is therefore

$$P_{\text{say}} = |\langle\psi_0|\psi_{k0}\rangle|^2 = \left| \int d^3\mathbf{r} e^{ikz} |\psi_0(\mathbf{r})|^2 \right|^2. \quad (15)$$

### 3

The two angular momentum degrees of freedom are the electron spin  $\mathbf{S}$  and the nucleus spin  $\mathbf{I}$ . Since we are at  $n = 0$ , the electron has no orbital angular momentum. The magnetic coupling Hamiltonian is

$$H_{\text{magnetic coupling}} = -\boldsymbol{\mu} \cdot \mathbf{B} = \frac{1}{\hbar} (2\mu_B \mathbf{S} - g_p \mu_N \mathbf{I}) \cdot \mathbf{B}. \quad (16)$$

Considering the component of  $\boldsymbol{\mu}$  along  $\mathbf{F} = \mathbf{S} + \mathbf{I}$  only, we have

$$H_{\text{magnetic coupling}} = \frac{1}{\hbar} \frac{(2\mu_B \mathbf{S} - g_p \mu_N \mathbf{I}) \cdot (\mathbf{S} + \mathbf{I})}{F^2} \mathbf{F} \cdot \mathbf{B}. \quad (17)$$

Expanding  $\mathbf{S}^2, \mathbf{I}^2$  and  $\mathbf{S} \cdot \mathbf{I}$ , we have

$$\frac{E}{m_F B} = \frac{1}{\hbar} \frac{2\mu_B S(S+1) - g_p \mu_N I(I+1) + (2\mu_B - g_p \mu_N) \cdot \frac{1}{2}(F(F+1) - S(S+1) - I(I+1))}{F(F+1)}. \quad (18)$$

Since we are working with hydrogen,  $I = 1/2$ ,  $S = 1/2$ , and  $F = 0, 1$ , and therefore

$$E = \frac{1}{\hbar} \frac{2\mu_B - g_p \mu_N}{2} m_F B. \quad (19)$$

So we have

$$E_{F=1, m_F} = E_0 + E_g + \frac{2\mu_B - g_p \mu_N}{2\hbar} m_F B, \quad (20)$$

and

$$E_{F=0, m_F=0} = E_0, \quad (21)$$

where  $E_0 = 13.6 \text{ eV}$ .

### 4

#### 4.1

The dipole interaction matrix is

$$H = -er\mathcal{E} \cos \theta. \quad (22)$$

When the initial state is

$$\psi_0(\mathbf{r}) = \frac{1}{\sqrt{\pi}} e^{-r}, \quad (23)$$

we have

$$E_0^{(1)} \propto \int d\Omega r^2 dr e^{-2r} r \propto \int_0^\infty r^3 e^{-2r} = 0 \quad (24)$$

by integration by parts.

#### 4.2