Notes and problems for Desai chapter III.

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1. Notes.

Chapter III notes and problems for [1].

FIXME: Some puzzling stuff in the interaction section and superposition of time-dependent states sections. Work through those here.

2. Problems

2.1. Problem 1. Virial Theorem.

2.1.1 Statement.

With the assumption that $\langle \mathbf{r} \cdot \mathbf{p} \rangle$ is independent of time, and

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) = T + V \tag{1}$$

show that

$$2\langle T\rangle = \langle \mathbf{r} \cdot \nabla V\rangle. \tag{2}$$

2.1.2 Solution.

I floundered with this a bit, but found the required hint in physicsforums. We can start with the Hamiltonian time derivative relation

$$i\hbar \frac{dA_H}{dt} = [A_H, H] \tag{3}$$

So, with the assumption that $\langle \mathbf{r} \cdot \mathbf{p} \rangle$ is independent of time, and the use of a stationary state $|\psi\rangle$ for the expectation calculation we have

$$0 = \frac{d}{dt} \langle \mathbf{r} \cdot \mathbf{p} \rangle$$

$$= \frac{d}{dt} \langle \psi | \mathbf{r} \cdot \mathbf{p} | \psi \rangle$$

$$= \langle \psi | \frac{d}{dt} (\mathbf{r} \cdot \mathbf{p}) | \psi \rangle$$

$$= \frac{1}{i\hbar} \langle [\mathbf{r} \cdot \mathbf{p}, H] \rangle$$

$$= - \left\langle \left[\mathbf{r} \cdot \nabla, \frac{\mathbf{p}^2}{2m} \right] \right\rangle - \left\langle [\mathbf{r} \cdot \nabla, V(\mathbf{r})] \right\rangle.$$

The exercise now becomes one of evaluating the remaining commutators. For the Laplacian commutator we have

$$\begin{bmatrix} \mathbf{r} \cdot \nabla, \nabla^2 \end{bmatrix} \psi = x_m \partial_m \partial_n \partial_n \psi - \partial_n \partial_n x_m \partial_m \psi$$

$$= x_m \partial_m \partial_n \partial_n \psi - \partial_n \partial_n \psi - \partial_n x_m \partial_n \partial_m \psi$$

$$= x_m \partial_m \partial_n \partial_n \psi - \partial_n \partial_n \psi - \partial_n \partial_n \psi - x_m \partial_n \partial_n \partial_m \psi$$

$$= -2 \nabla^2 \psi$$

For the potential commutator we have

$$[\mathbf{r} \cdot \nabla, V(\mathbf{r})] \psi = x_m \partial_m V \psi - V x_m \partial_m \psi$$

$$= x_m (\partial_m V) \psi x_m V \partial_m \psi - V x_m \partial_m \psi$$

$$= (\mathbf{r} \cdot (\nabla V)) \psi$$

Putting all the \hbar factors back in, we get

$$2\left\langle \frac{\mathbf{p}^2}{2m}\right\rangle = \left\langle \mathbf{r} \cdot (\nabla V)\right\rangle,\tag{4}$$

which is the desired result.

Followup: why assume $\langle \mathbf{r} \cdot \mathbf{p} \rangle$ is independent of time?

2.2. Problem 2. Application of virial theorem.

Calculate $\langle T \rangle$ with $V = \lambda \ln(r/a)$.

$$\mathbf{r} \cdot \nabla V = r\hat{\mathbf{r}} \cdot \hat{\mathbf{r}} \lambda \frac{\partial \ln(r/a)}{\partial r}$$

$$= \lambda r \frac{1}{a} \frac{a}{r}$$

$$= \lambda$$

$$\Longrightarrow$$

$$\langle T \rangle = \lambda/2$$

2.3. Problem 3. Heisenberg Position operator representation.

2.3.1 Part I.

Express x as an operator x_H for $H = \mathbf{p}^2/2m$. With

$$\langle \psi | x | \psi \rangle = \langle \psi_0 | U^{\dagger} x U | \psi_0 \rangle$$

We want to expand

$$\begin{aligned} x_{H} &= U^{\dagger} x U \\ &= e^{iHt/\hbar} x e^{-iHt/\hbar} \\ &= \sum_{k,l=0}^{\infty} \frac{1}{k!} \frac{1}{l!} \left(\frac{iHt}{\hbar} \right)^{k} x \left(\frac{-iHt}{\hbar} \right)^{l}. \end{aligned}$$

We to evaluate $H^k x H^l$ to proceed. Using $p^n x = -i\hbar n p^{n-1} + x p^n$, we have

$$H^{k}x = \frac{1}{(2m)^{k}} p^{2}kx$$

$$= \frac{1}{(2m)^{k}} \left(-i\hbar(2k) p^{2k-1} + xp^{2}k \right)$$

$$= xH^{k} + \frac{1}{2m} (-i\hbar)(2k) pp^{2(k-1)} / (2m)^{k-1}$$

$$= xH^{k} - \frac{i\hbar k}{m} pH^{k-1}.$$

This gives us

$$x_{H} = x - \frac{i\hbar p}{m} \sum_{k,l=0}^{\infty} \frac{k}{k!} \frac{1}{l!} \left(\frac{it}{\hbar}\right)^{k} H^{k-1+l} \left(\frac{-it}{\hbar}\right)^{l}$$
$$= x - \frac{i\hbar pit}{m\hbar}$$

Or

$$x_H = x + \frac{pt}{m} \tag{5}$$

2.3.2 Part II.

Express x as an operator x_H for $H = \mathbf{p}^2/2m + V$ with $V = \lambda x^m$.

In retrospect, for the first part of this problem, it would have been better to use the series expansion for this exponential sandwich

Or, in explicit form

$$e^{A}Be^{-A} = B + \frac{1}{1!}[A, B] + \frac{1}{2!}[A, [A, B]] + \cdots$$
 (6)

Doing so, we'd find for the first commutator

$$\frac{it}{2m\hbar} \left[\mathbf{p}^2, x \right] = \frac{tp}{m},\tag{7}$$

so that the series has only the first two terms, and we'd obtain the same result. That seems like a logical approach to try here too. For the first commutator, we get the same tp/m result since [V,x]=0.

Employing

$$x^n p = i\hbar n x^{n-1} + p x^n, \tag{8}$$

I find

$$\left(\frac{it}{\hbar}\right)^{2} [H, [H, x]] = \frac{i\lambda t^{2}}{\hbar m} [x^{n}, p]$$

$$= -\frac{nt^{2}\lambda}{m} x^{n-1}$$

$$= -\frac{nt^{2}V}{mx}$$

The triple commutator gets no prettier, and I get

$$\left(\frac{it}{\hbar}\right)^{3} [H, [H, [H, x]]] = \frac{it}{\hbar} \left[\frac{\mathbf{p}^{2}}{2m} + \lambda x^{n}, -\frac{nt^{2}V}{mx}\right]$$

$$= -\frac{it}{\hbar} \frac{nt^{2}}{m} \frac{\lambda}{2m} \left[\mathbf{p}^{2}, x^{n-1}\right]$$

$$= \cdots$$

$$= \frac{n(n-1)t^{3}V}{2m^{2}x^{3}} (i\hbar n + 2px).$$

Putting all the pieces together this gives

$$x_H = e^{iHt/\hbar} x e^{-iHt/\hbar} = x + \frac{tp}{m} - \frac{nt^2V}{2mx} + \frac{n(n-1)t^3V}{12m^2x^3} (i\hbar n + 2px) + \cdots$$
 (9)

If there is a closed form for this it isn't obvious to me. Would a fixed lower degree potential function shed any more light on this. How about the Harmonic oscillator Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2 \tag{10}$$

... this one works out nicely since there's an even-odd alternation. Get

$$x_H = x\cos(\omega^2 t^2/2) + \frac{pt}{m} \frac{\sin(\omega^2 t^2/2)}{\omega^2 t^2/2}$$
 (11)

I'd not expect such a tidy result for an arbitrary $V(x) = \lambda x^n$ potential.

2.4. Problem 4. Feynman-Hellman relation.

For continuously parametrized eigenstate, eigenvalue and Hamiltonian $|\psi(\lambda)\rangle$, $E(\lambda)$ and $H(\lambda)$ respectively, we can relate the derivatives

$$\frac{\partial}{\partial \lambda}(H|\psi\rangle) = \frac{\partial}{\partial \lambda}(E|\psi\rangle)$$

$$\Longrightarrow$$

$$\frac{\partial H}{\partial \lambda}|\psi\rangle + H\frac{\partial|\psi\rangle}{\partial \lambda} = \frac{\partial E}{\partial \lambda}|\psi\rangle + E\frac{\partial|\psi\rangle}{\partial \lambda}$$

Left multiplication by $\langle \psi |$ gives

$$\langle \psi | \frac{\partial H}{\partial \lambda} | \psi \rangle + \langle \psi | H \frac{\partial | \psi \rangle}{\partial \lambda} = \langle \psi | \frac{\partial E}{\partial \lambda} | \psi \rangle + E \langle \psi | \frac{\partial | \psi \rangle}{\partial \lambda}$$

$$\Longrightarrow$$

$$\langle \psi | \frac{\partial H}{\partial \lambda} | \psi \rangle + (\langle \psi | E) \frac{\partial | \psi \rangle}{\partial \lambda} = \langle \psi | \frac{\partial E}{\partial \lambda} | \psi \rangle + E \langle \psi | \frac{\partial | \psi \rangle}{\partial \lambda}$$

$$\Longrightarrow$$

$$\langle \psi | \frac{\partial H}{\partial \lambda} | \psi \rangle = \frac{\partial E}{\partial \lambda} \langle \psi | \psi \rangle ,$$

which provides the desired identity

$$\frac{\partial E}{\partial \lambda} = \langle \psi(\lambda) | \frac{\partial H}{\partial \lambda} | \psi(\lambda) \rangle \tag{12}$$

2.5. **Problem 5.**

2.5.1 Description.

With eigenstates $|\phi_1\rangle$ and $|\phi_2\rangle$, of H with eigenvalues E_1 and E_2 , respectively, and

$$egin{aligned} |\chi_1
angle &= rac{1}{\sqrt{2}}(|\phi_1
angle + |\phi_2
angle) \ |\chi_2
angle &= rac{1}{\sqrt{2}}(|\phi_1
angle - |\phi_2
angle) \end{aligned}$$

and $|\psi(0)\rangle = |\chi_1\rangle$, determine $|\psi(t)\rangle$ in terms of $|\phi_1\rangle$ and $|\phi_2\rangle$.

2.5.2 Solution.

$$\begin{aligned} |\psi(t)\rangle &= e^{-iHt/\hbar} |\psi(0)\rangle \\ &= e^{-iHt/\hbar} |\chi_1\rangle \\ &= \frac{1}{\sqrt{2}} e^{-iHt/\hbar} (|\phi_1\rangle - |\phi_2\rangle) \\ &= \frac{1}{\sqrt{2}} (e^{-iE_1t/\hbar} |\phi_1\rangle - e^{-iE_2t/\hbar} |\phi_2\rangle) \end{aligned} \quad \Box$$

2.6. **Problem 6.**

2.6.1 Description.

Consider a Coulomb like potential $-\lambda/r$ with angular momentum l=0. If the eigenfunction is

$$u(r) = u_0 e^{-\beta r} \tag{13}$$

determine u_0 , β , and the energy eigenvalue E in terms of λ , and m.

2.6.2 Solution.

We can start with the normalization constant u_0 by integrating

$$1 = u_0^2 \int_0^\infty dr e^{-\beta r} e^{-\beta r}$$
$$= u_0^2 \left. \frac{e^{-2\beta r}}{-2\beta} \right|_{0^\infty}$$
$$= u_0^2 \frac{1}{2\beta}$$

$$u_0 = \sqrt{2\beta} \tag{14}$$

To go further, we need the Hamiltonian. Note that we can write the Laplacian with the angular momentum operator factored out using

$$\nabla^2 = \frac{1}{\mathbf{x}^2} \left((\mathbf{x} \cdot \nabla)^2 + \mathbf{x} \cdot \nabla + (\mathbf{x} \times \nabla)^2 \right)$$
 (15)

With zero for the angular momentum operator $\mathbf{x} \times \nabla$, and switching to spherical coordinates, we have

$$\nabla^2 = \frac{1}{r}\partial_r + \frac{1}{r}\partial_r r\partial_r$$

$$= \frac{1}{r}\partial_r + \frac{1}{r}\partial_r + \frac{1}{r}r\partial_{rr}$$

$$= \frac{2}{r}\partial_r + \partial_{rr}$$

We can now write the Hamiltonian for the zero angular momentum case

$$H = -\frac{\hbar^2}{2m} \left(\frac{2}{r} \partial_r + \partial_{rr} \right) - \frac{\lambda}{r} \tag{16}$$

With application of this Hamiltonian to the eigenfunction we have

$$Eu_0e^{-\beta r} = \left(-\frac{\hbar^2}{2m}\left(\frac{2}{r}\partial_r + \partial_{rr}\right) - \frac{\lambda}{r}\right)u_0e^{-\beta r}$$
$$= \left(-\frac{\hbar^2}{2m}\left(\frac{2}{r}(-\beta) + \beta^2\right) - \frac{\lambda}{r}\right)u_0e^{-\beta r}.$$

In particular for $r = \infty$ we have

$$-\frac{\hbar^2 \beta^2}{2m} = E \tag{17}$$

$$-\frac{\hbar^2 \beta^2}{2m} = \left(-\frac{\hbar^2}{2m} \left(\frac{2}{r}(-\beta) + \beta^2\right) - \frac{\lambda}{r}\right)$$

$$\Longrightarrow$$

$$\frac{\hbar^2}{2m} \frac{2}{r} \beta = \frac{\lambda}{r}$$

Collecting all the results we have

$$\beta = \frac{\lambda m}{\hbar^2} \tag{18}$$

$$E = -\frac{\lambda^2 m}{2\hbar^2} \tag{19}$$

$$u_0 = \frac{\sqrt{2\lambda m}}{\hbar} \tag{20}$$

2.7. **Problem 7.**

2.7.1 Description.

A particle in a uniform field E_0 . Show that the expectation value of the position operator $\langle r \rangle$ satisfies

$$m\frac{d^2\langle \mathbf{r}\rangle}{dt^2} = e\mathbf{E}_0. \tag{21}$$

2.7.2 Solution.

This follows from Ehrehfest's theorem once we formulate the force $e\mathbf{E}_0 = -\nabla \phi$, in terms of a potential ϕ . That potential is

$$\phi = -e\mathbf{E}_0 \cdot (x, y, z) \tag{22}$$

The Hamiltonian is therefore

$$H = \frac{\mathbf{p}^2}{2m} - e\mathbf{E}_0 \cdot (x, y, z). \tag{23}$$

Ehrehfest's theorem gives us

$$\frac{d}{dt} \langle x_k \rangle = \frac{1}{m} \langle p_k \rangle$$

$$\frac{d}{dt} \langle p_k \rangle = -\left\langle \frac{\partial V}{\partial x_k} \right\rangle,$$

or

$$\frac{d^2}{dt^2} \langle x_k \rangle = -\frac{1}{m} \left\langle \frac{\partial V}{\partial x_k} \right\rangle. \tag{24}$$

$$\frac{\partial V}{\partial x_k} = -e(\mathbf{E}_0)_k$$

Putting all the last bits together, and summing over the directions \mathbf{e}_k we have

$$m\frac{d^2}{dt^2}\mathbf{e}_k \langle x_k \rangle = \mathbf{e}_k \langle e(\mathbf{E}_0)_k \rangle = e\mathbf{E}_0 \qquad \Box$$

2.8. **Problem 8.**

2.8.1 Description.

For Hamiltonian eigenstates $|E_n\rangle$, C=AB, A=[B,H], obtain the matrix element $\langle E_m|C|E_n\rangle$ in terms of the matrix element of A.

2.8.2 Solution.

I was able to get most of what was asked for here, with a small exception. I started with the matrix element for *A*, which is

$$\langle E_m | A | E_n \rangle = \langle E_m | BH - HB | E_n \rangle = (E_n - E_m) \langle E_m | B | E_n \rangle \tag{25}$$

Next, computing the matrix element for *C* we have

$$\langle E_m | C | E_n \rangle = \langle E_m | BHB - HB^2 | E_n \rangle$$

$$= \sum_a \langle E_m | BH | E_a \rangle \langle E_a | B | E_n \rangle - E_m \langle E_m | B | E_a \rangle \langle E_a | B | E_n \rangle$$

$$= \sum_a E_a \langle E_m | B | E_a \rangle \langle E_a | B | E_n \rangle - E_m \langle E_m | B | E_a \rangle \langle E_a | B | E_n \rangle$$

$$= \sum_a \langle E_a - E_m \rangle \langle E_m | B | E_a \rangle \langle E_a | B | E_n \rangle$$

$$= \sum_a \langle E_m | A | E_a \rangle \langle E_a | B | E_n \rangle$$

$$= \langle E_m | A | E_n \rangle \langle E_n | B | E_n \rangle + \sum_{a \neq n} \langle E_m | A | E_a \rangle \langle E_a | B | E_n \rangle$$

$$= \langle E_m | A | E_n \rangle \langle E_n | B | E_n \rangle + \sum_{a \neq n} \langle E_m | A | E_a \rangle \frac{\langle E_a | A | E_n \rangle}{E_n - E_a}$$

Except for the $\langle E_n|B|E_n\rangle$ part of this expression, the problem as stated is complete. The relationship 25 is no help for with n=m, so I see no choice but to leave that small part of the expansion in terms of B.

2.9. **Problem 9.**

2.9.1 Description.

Operator A has eigenstates $|a_i\rangle$, with a unitary change of basis operation $U|a_i\rangle=|b_i\rangle$. Determine in terms of U, and A the operator B and its eigenvalues for which $|b_i\rangle$ are eigenstates.

2.9.2 Solution.

Consider for motivation the matrix element of A in terms of $|b_i\rangle$. We will also let $A|a_i\rangle=\alpha_i|a_i\rangle$. We then have

$$\langle a_i|A|a_j\rangle = \langle b_i|UAU^{\dagger}|b_j\rangle$$

We also have

$$\langle a_i | A | a_j \rangle = a_j \langle a_i | | a_j \rangle$$

= $a_i \delta_{ii}$

So it appears that the operator UAU^{\dagger} has the orthonormality relation required. In terms of action on the basis $\{|b_i\rangle\}$, let's see how it behaves. We have

$$UAU^{\dagger}|b_{i}\rangle = UA|a_{i}\rangle$$

= $U\alpha_{i}|a_{i}\rangle$
= $\alpha_{i}|b_{i}\rangle$

So we see that the operators A and $B = UAU^{\dagger}$ have common eigenvalues.

2.10. Problem 10.

2.10.1 Description.

With $H|n\rangle = E_n|n\rangle$, A = [H, F] and $\langle 0|F|0\rangle = 0$, show that

$$\sum_{n \neq 0} \frac{\langle 0|A|n\rangle\langle n|A|0\rangle}{E_n - E_0} = \langle 0|AF|0\rangle \tag{26}$$

2.10.2 Solution.

$$\langle 0|AF|0\rangle = \langle 0|HFF - FHF|0\rangle$$

$$= \sum_{n} E_{0}\langle 0|F|n\rangle\langle n|F|0\rangle - E_{n}\langle 0|F|n\rangle\langle n|F|0\rangle$$

$$= \sum_{n} (E_{0} - E_{n})\langle 0|F|n\rangle\langle n|F|0\rangle$$

$$= \sum_{n\neq 0} (E_{0} - E_{n})\langle 0|F|n\rangle\langle n|F|0\rangle$$

We also have

$$\langle 0|A|n\rangle\langle n|A|0\rangle = \langle 0|HF - FH|n\rangle\langle n|A|0\rangle$$

$$= (E_0 - E_n)\langle 0|F|n\rangle\langle n|HF - FH|0\rangle$$

$$= -(E_0 - E_n)^2\langle 0|F|n\rangle\langle n|F|0\rangle$$

Or, for $n \neq 0$,

$$\langle 0|F|n\rangle\langle n|F|0\rangle = -\frac{\langle 0|A|n\rangle\langle n|A|0\rangle}{(E_0 - E_n)^2}.$$

This gives

$$\langle 0|AF|0\rangle = -\sum_{n\neq 0} (E_0 - E_n) \frac{\langle 0|A|n\rangle \langle n|A|0\rangle}{(E_0 - E_n)^2}$$
$$= \sum_{n\neq 0} \frac{\langle 0|A|n\rangle \langle n|A|0\rangle}{E_n - E_0} \quad \Box$$

2.11. Problem 11. commutator of angular momentum with Hamiltonian.

Show that $[\mathbf{L}, H] = 0$, where $H = \mathbf{p}^2/2m + V(r)$. This follows by considering $[\mathbf{L}, \mathbf{p}^2]$, and $[\mathbf{L}, V(r)]$. Let

$$L_{ik} = x_i p_k - x_k p_i, (27)$$

so that

$$\mathbf{L} = \mathbf{e}_i \epsilon_{ijk} L_{jk}. \tag{28}$$

We now need to consider the commutators of the operators L_{jk} with \mathbf{p}^2 and V(r). Let's start with p^2 . In particular

$$\mathbf{p}^{2}x_{m}p_{n} = p_{k}p_{k}x_{m}p_{n}$$

$$= p_{k}(p_{k}x_{m})p_{n}$$

$$= p_{k}(-i\hbar\delta_{km} + x_{m}p_{k})p_{n}$$

$$= -i\hbar p_{m}p_{n} + (p_{k}x_{m})p_{k}p_{n}$$

$$= -i\hbar p_{m}p_{n} + (-i\hbar\delta_{km} + x_{m}p_{k})p_{k}p_{n}$$

$$= -2i\hbar p_{m}p_{n} + x_{m}p_{n}\mathbf{p}^{2}.$$

So our commutator with p^2 is

$$[L_{ik}, \mathbf{p}^2] = (x_i p_k - x_i p_k) \mathbf{p}^2 - (-2i\hbar p_i p_k + x_i p_k \mathbf{p}^2 + 2i\hbar p_k p_i - x_k p_i \mathbf{p}^2).$$

Since $p_i p_k = p_k p_j$, all terms cancel out, and the problem is reduced to showing that

$$[L, H] = [L, V(r)] = 0.$$

Now assume that V(r) has a series representation

$$V(r) = \sum_{j} a_j r^j = \sum_{j} a_j (x_k x_k)^{j/2}$$

We'd like to consider the action of $x_m p_n$ on this function

$$\begin{aligned} x_m p_n V(r) \Psi &= -i\hbar x_m \sum_j a_j \partial_n (x_k x_k)^{j/2} \Psi \\ &= -i\hbar x_m \sum_j a_j (j x_n (x_k x_k)^{j/2-1} + r^j \partial_n \Psi) \\ &= -\frac{i\hbar x_m x_n}{r^2} \sum_j a_j j r^j + x_m V(r) p_n \Psi \end{aligned}$$

$$L_{mn}V(r) = (x_{m}p_{n} - x_{n}p_{m})V(r)$$

$$= -\frac{i\hbar x_{m}x_{n}}{r^{2}} \sum_{j} a_{j}jr^{j} + \frac{i\hbar x_{n}x_{m}}{r^{2}} \sum_{j} a_{j}jr^{j} + V(r)(x_{m}p_{n} - x_{n}p_{m})$$

$$= V(r)L_{mn}$$

Thus $[L_{mn}, V(r)] = 0$ as expected, implying $[\mathbf{L}, H] = 0$.

References

 $[1] \ \ BR \ Desai. \ \textit{Quantum mechanics with basic field theory}. \ Cambridge \ University \ Press, 2009. \ \textbf{1}$