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Quantum Mechanics B (Physics 212B) Winter 2019
Worksheet 7 – Solutions

Problems

1. **TRK Sum Rule: Generalized**

   Consider an atom with Z electrons, and Hamiltonian

$$H = \sum_{k=1}^{Z} \frac{\mathbf{p}_k^2}{2m} + V(\mathbf{r}_1, \ldots, \mathbf{r}_Z) \tag{1}$$

   Let $r_{a,s}$ denote coordinate a of electron s, so that $r_{1,s} \equiv x_s$ is the x coordinate of electron s, etc. Compute the matrix element

$$\langle i \,|\, [[r_{a,s}, H]\,, r_{b,k}] \,|\, i\rangle \tag{2}$$

   in two different ways — (a) by inserting a complete set of states (b) by computing the commutators using the Hamiltonian Eq. (1) to prove the Thomas-Reiche-Kuhn sum rule:

$$\frac{\hbar^2}{m}\delta_{sk}\delta_{ab} = \sum_j (E_j - E_i)\left[\langle i|r_{a,s}|j\rangle \langle j|r_{b,k}|i\rangle + \langle i|r_{b,k}|j\rangle \langle j|r_{a,s}|i\rangle\right] \tag{3}$$

$$\begin{aligned} [[r_{a,s}, H]\,, r_{b,k}] &= [r_{a,s}H - Hr_{a,s}, r_{b,k}] \\ &= r_{a,s}Hr_{b,k} + r_{b,k}Hr_{a,s} - Hr_{a,s}r_{b,k} - r_{b,k}r_{a,s}H \end{aligned} \tag{4}$$

   Taking the $\langle i| \cdot |i\rangle$ matrix element of Eq. (4) and inserting a complete set of states

$$\begin{aligned} \langle i|\,[[r_{a,s}, H]\,, r_{b,k}]\,|i\rangle &= \sum_j \Big[\langle i|r_{a,s}H|j\rangle \langle j|r_{b,k}|i\rangle + \langle i|r_{b,k}H|j\rangle \langle j|r_{a,s}|i\rangle \\ &\quad - \langle i|Hr_{a,s}|j\rangle \langle j|r_{b,k}|i\rangle - \langle i|r_{b,k}|j\rangle \langle j|r_{a,s}H|i\rangle\Big] \\ &= \sum_j (E_j - E_i)\left[\langle i|r_{a,s}|j\rangle \langle j|r_{b,k}|i\rangle + \langle i|r_{b,k}|j\rangle \langle j|r_{a,s}|i\rangle\right] \end{aligned} \tag{5}$$

   since the states are eigenstates of H.,

$$\begin{aligned} [r_{a,s}, H] &= \frac{i\hbar p_{a,s}}{m} \\ [[r_{a,s}, H]\,, r_{b,k}] &= \frac{\hbar^2}{m}\delta_{sk}\delta_{ab} \end{aligned} \tag{6}$$

so that

$$\frac{\hbar^2}{m}\delta_{sk}\delta_{ab} = \sum_j (E_j - E_i)\left[\langle i|r_{a,s}|j\rangle \langle j|r_{b,k}|i\rangle + \langle i|r_{b,k}|j\rangle \langle j|r_{a,s}|i\rangle\right] \tag{7}$$

2. **Energy Loss of a Charged Particle**

A charged particle with charge $Z_p e$ passes by a stationary atom. This problem computes the energy lost by the charged particle to the atom. For the calculation, assume the particle moves in a straight-line trajectory $\mathbf{R}(t)$ with velocity v and impact parameter b, and compute the mean excitation energy of the atom.

(a) Write down the perturbing potential to the kth-electron due to the external charge. Assuming a large impact parameter $b \gg \langle \vec{r}_k \rangle$ expand the potential to first order in $|\frac{\vec{r}_k}{\mathbf{R}}|$

The interaction Hamiltonian is

$$H_{\text{int}}(t) = -\sum_k \frac{Z_p e^2}{|\mathbf{R}(t) - \mathbf{r}_k|} \tag{8}$$

Since $|\mathbf{R}(t)| \gg |\mathbf{r}_i|$,

$$\frac{1}{|\mathbf{R}(t) - \mathbf{r}_k|} \approx \frac{1}{|\mathbf{R}(t)|} + \frac{\mathbf{r}_k \cdot \mathbf{R}(t)}{|\mathbf{R}(t)|^3} + \dots \tag{9}$$

The first term produces an irrelevant shift to the ground-state energy, so we can ignore it.

We can then write the interaction Hamiltonian as:

$$H_{\text{int}}(t) \approx -Z_p e^2 \sum_k \frac{\mathbf{r}_k \cdot \mathbf{R}(t)}{|\mathbf{R}(t)|^3} \tag{10}$$

(b) Suppose a transition occurs of the k-th electron from $|i\rangle \to |f\rangle$ with $E_f \neq E_i$. Calculate to first order in time-dependent perturbation theory the amplitude for this transition as $t \to \infty$. You may assume the frequency of the transition is small compared to the timescale it happens on. The answer will be in terms of matrix elements of $\vec{r}_k$

To first order, the amplitude to make a transition $|i\rangle \to |f\rangle$ is

$$A_{fi} = -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt\ \langle f|H_{\text{int}}(t)|i\rangle\, e^{i\omega_{fi}t} \tag{11}$$

where $\hbar\omega_{fi} = E_f - E_i$. The condition of a fast particle implies that $\omega_{fi}t \ll 1$, so

$$A_{fi} \approx -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt\, \langle f|H_{\text{int}}(t)|i\rangle \tag{12}$$

Assuming the results above we plug in:

$$A_{fi}(t) \approx \frac{iZ_pe^2}{\hbar} \sum_k \int_{-\infty}^{\infty} dt \, \langle f| \frac{\mathbf{r}_k \cdot \mathbf{R}(t)}{|\mathbf{R}(t)|^3} |i\rangle = \frac{iZ_pe^2}{\hbar} \int_{-\infty}^{\infty} dt \frac{\mathbf{R}(t)}{|\mathbf{R}(t)|^3} \cdot \sum_k \langle f|\mathbf{r}_k|i\rangle \tag{13}$$

Choosing the incident particle to have impact parameter b in the $\mathbf{x}$ direction, and moving with velocity v in the $\mathbf{z}$ direction,

$$\mathbf{R}(t) = b\hat{\mathbf{x}} + vt\hat{\mathbf{z}} \tag{14}$$

and

$$\mathbf{I} = \int_{-\infty}^{\infty} dt \frac{\mathbf{R}(t)}{|\mathbf{R}(t)|^3} = \int_{-\infty}^{\infty} dt \frac{b\hat{\mathbf{x}} + vt\hat{\mathbf{z}}}{(b^2 + v^2t^2)^{3/2}} \tag{15}$$

Let

$$\tan\theta(t) = \frac{vt}{b} \tag{16}$$

so that

$$\begin{aligned} \mathbf{I} = &= \int_{-\infty}^{\infty} \frac{b\hat{\mathbf{x}} + b\tan\theta\hat{\mathbf{z}}}{b^3\sec^3\theta} \frac{b}{v} \sec^2\theta \, d\theta \\ &= \frac{1}{bv} \left[\sin\theta\hat{\mathbf{x}} - \cos\theta\hat{\mathbf{z}}\right]_{-\pi/2}^{\pi/2} \\ &= \frac{2}{bv}\hat{\mathbf{x}} \end{aligned} \tag{17}$$

and

$$A_{fi}(t) = \frac{2iZ_pe^2}{bv\hbar} \sum_k \langle f|x_k|i\rangle \tag{18}$$

(c) Write the average energy loss as a weighted sum of energy differences times probabilities of the associated transitions. Using the above result and the TRK sum rule, calculate this.

The energy loss is given by weighting the final state probabilities with the excitation energy,

$$\begin{aligned} E = \sum_f (E_f - E_i) |A_{fi}|^2 &= \frac{4Z_p^2e^4}{b^2v^2\hbar^2} \sum_f (E_f - E_i) \left|\sum_k \langle f|x_k|i\rangle\right|^2 \\ &= \frac{4Z_p^2e^4}{b^2v^2\hbar^2} \sum_{k,r} \sum_f (E_f - E_i) \langle i|x_r|f\rangle \langle f|x_k|i\rangle \end{aligned} \tag{19}$$

Note the subscript on x is the particle label, not the coordinate label $1, 2, 3$. Using the Thomas-Reiche-Kuhn sum rule,

$$\sum_{k,r} \sum_f (E_f - E_i) \langle i|x_r|f\rangle \langle f|x_k|i\rangle = \frac{1}{2} \sum_{k,r} \sum_f (E_f - E_i) \left[\langle i|x_r|f\rangle \langle f|x_k|i\rangle + \langle i|x_k|f\rangle \langle f|x_r|i\rangle\right]$$
$$= \sum_{kr} \frac{\hbar^2}{2m} \delta_{kr} = \frac{\hbar^2}{2m} Z \tag{20}$$

where Z is the number of electrons in the atom. Then the energy loss Eq. (**??**) is

$$E = \frac{2Z_p^2 Z e^4}{b^2 v^2 m} \tag{21}$$

Note the result goes as Z_p^2 but is linear in Z. The electrons are excited incoherently, i.e. the energy loss is proportional to the number of electrons.