Quantum mechanics 2 practical course Supplementary test 1 Nov 12^{th}, 2021

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1. **Problem** 25 points

Two electrons interact with contact potential:

$$H(1,2) = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \gamma\delta(x_1 - x_2) \; .$$

a) Introduce the new coordinates $X = \frac{x_1+x_2}{2}$ and $x = x_2 - x_1$ and rewrite the Hamilton operator of the two particles!

b) Solve the stationary Schrödinger equation for the bound state (square integrable eigenfunction) of the system! Give the spin-part of the wavefunction!

c) Give the condition that the bound state has a negative energy!

Supporting information: Boundary condition for the Dirac-delta

$$\psi'(0+) - \psi'(0-) = -\frac{m\gamma}{\hbar^2}\psi(0)$$

Solution:

(a) The new momenta corresponding to $X = x_1 + x_2,\; mathcalP = \frac{\hbar}{i}\frac{\partial}{\partial X}$ and $x = x_2 - x_1,\; p = \frac{\hbar}{i}\frac{\partial}{\partial x}$

$$p_1 = \frac{\hbar}{i}\frac{\partial}{\partial x_1} = \frac{\hbar}{i}\left(\frac{\partial X}{\partial x_1}\frac{\partial}{\partial X} + \frac{\partial x}{\partial x_1}\frac{\partial}{\partial x}\right) = \frac{\mathcal{P}}{2} - p \tag{1}$$

$$p_2 = \frac{\hbar}{i}\frac{\partial}{\partial x_2} = \frac{\hbar}{i}\left(\frac{\partial X}{\partial x_2}\frac{\partial}{\partial X} + \frac{\partial x}{\partial x_2}\frac{\partial}{\partial x}\right) = \frac{\mathcal{P}}{2} + p \tag{2}$$

$$\Rightarrow \mathcal{P} = p_1 + p_2, \;\; p = \frac{p_2 - p_1}{2} \tag{3}$$

With these new variables the Hamiltonian takes the form:

$$H = \frac{\mathcal{P}^2}{4m} + \frac{p^2}{m} - \gamma\delta(x) \tag{4}$$

corresponding to a free particle with mass $2m$ and a particle with a Dirac-delta potential with mass $\frac{m}{2}$.

(b) Writing in the original coordiantes the wave function takes the form:

$$\Psi(x_1, x_2) = \varphi(x_1 + x_2)\psi(x_2 - x_1) \sim e^{ik(x_1+x_2) - \alpha|x_2 - x_1|} \tag{5}$$

being symmetric in x_1 and x_2, that is in order to have a antisymmetric total wavefunction we need an antisymmetric singlet spinor part, $|0,0\rangle$:

$$\Phi(x_1, x_2, s_1, s_2) = \Psi(x_1, x_2)|0,0\rangle \tag{6}$$

having a total spin of zero!

(c) The bound state is the one when the particle in the Dirac delta potential has negative energy, $E = -|E|$:

$$\partial_x^2\psi(x) = \frac{2m|E|}{\hbar^2}\psi(x) \tag{7}$$

$$\psi'(0+) - \psi'(0-) = -\frac{m\gamma}{\hbar^2}\psi(0) \tag{8}$$

The solution of this is $Ae^{-\alpha|x|}$, with $\alpha = \sqrt{\frac{m|E|}{\hbar^2}} = \frac{m\gamma}{2\hbar^2} \to E = -\frac{m\gamma^2}{4\hbar^2}$ and $A = \sqrt{\frac{1}{2\alpha}}$. While for the other particle we have the usual free solution:

$$\varphi(X) = Be^{ikX}, \quad k = 2\sqrt{\frac{mE_2}{\hbar^2}} \tag{9}$$

with $E_2 > 0$. The negativity of $E_2 + E < 0 \Leftrightarrow \frac{k^2\hbar^2}{4m} < \frac{m\gamma^2}{4\hbar^2} \to k < \frac{m\gamma}{\hbar^2}$!

2. **Problem** 25 points

In the ground state of a Na atom the single valence electron occupies one of the $3s$ ($L = 0$) orbitals, while the first excited states are the $3p$ ($L = 1$) orbitals.

a) In the first excited state, the total angular momentum operator $\vec{J} = \vec{L} + \vec{S}$ can have the quantum numbers $J = \frac{1}{2}$ and $J = \frac{3}{2}$. Consider a static perturbation $H_1 = \alpha\vec{L}\vec{S}$ (spin-orbit coupling)! Calculate the energy difference between the states for $J = \frac{1}{2}$ and $J = \frac{3}{2}$!

Hint: Express the $\vec{L}\vec{S}$ operator with the help of the operators $\vec{J}^2 = (\vec{L} + \vec{S})^2$, $\vec{L}^2$ and $\vec{S}^2$!

b) A harmonic perturbation of frequency ω,

$$V(t) = \mathcal{E}ez\cos(\omega t)\,,$$

is applied, where $\mathcal{E}$ denotes a uniform electric field along the z direction and e is the unit charge. Find the excited states $|J = \frac{1}{2}, M_J\rangle$ to which a transition is allowed from the ground state $|L, M\rangle|S, M_S\rangle = |0,0\rangle|\frac{1}{2}, \frac{1}{2}\rangle$ within first order time-dependent perturbation theory!

Supporting information: the transition matrix element is defined as $\langle\varphi_1|V|\varphi_0\rangle = \mathcal{E}e\,\langle\varphi_1|z|\varphi_0\rangle$, $z = r\sqrt{\frac{4\pi}{3}}Y_1^0 = r\sqrt{\frac{4\pi}{3}}|1,0\rangle$

Solution:

(a) The total spin $J = L + S$ in the $L = 1$ subspace, according to the Clebsh-Gordan rules, can be $J = 3/2, 1/2$, while in the $L = 0$ subspace it is simply $J = 1/2$. Giving an energy The product can be expressed as $\frac{\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2}{2}$ having possible eigenvalues of $\frac{15/4 - 2 - 3/4}{2}\hbar^2 = \hbar^2/2$ for $J = 3/2$ and $\frac{3/4 - 2 - 3/4}{2}\hbar^2 = -\hbar^2$ for $J = 1/2$, giving the energy difference $\alpha\frac{3}{2}\hbar^2$

(b) Nevertheless, we actually do not need the Clebsh Gordan coefficients, for sake of extra practice we give them for $L = 1$ where we have 6 different states:

$$|1/2, 1/2\rangle = \frac{1}{\sqrt{3}}|1,0\rangle|1/2, 1/2\rangle - \sqrt{\frac{2}{3}}|1,1\rangle|1/2, -1/2\rangle \tag{10}$$

$$|1/2, -1/2\rangle = \sqrt{\frac{2}{3}}|1,0\rangle|1/2, -1/2\rangle - \frac{1}{\sqrt{3}}|1,-1\rangle|1/2, 1/2\rangle \tag{11}$$

$$|3/2, 3/2\rangle = |1,1\rangle|1/2, 1/2\rangle \tag{12}$$

$$|3/2, 1/2\rangle = \sqrt{\frac{2}{3}}|1,0\rangle|1/2, 1/2\rangle + \frac{1}{\sqrt{3}}|1,1\rangle|1/2, -1/2\rangle \tag{13}$$

$$|3/2, -1/2\rangle = \frac{1}{\sqrt{3}}|1,0\rangle|1/2, -1/2\rangle + \sqrt{\frac{2}{3}}|1,-1\rangle|1/2, 1/2\rangle \tag{14}$$

$$|3/2, -3/2\rangle = |1,-1\rangle|1/2, -1/2\rangle \tag{15}$$

The spatial part of the ground state is just a constant as $L = 0$ we can consider the $z|\varphi_0\rangle$ term in the inner product as $|1,0\rangle|1/2, \pm 1/2\rangle$ Now we only need to know what $M_J$quantum numbers can come up in the $J = 1/2$ subspace

$$\langle 1/2, 1/2| \rangle \neq 0 = \left(= \frac{1}{\sqrt{3}}\right) \tag{16}$$

$$\langle 3/2, 1/2|1,0\rangle|1/2,1/2\rangle \neq 0 \left(= \sqrt{\frac{2}{3}}\right) \tag{17}$$

$$\langle 3/2, -1/2|1,0\rangle|1/2,-1/2\rangle \neq 0 \left(= \frac{1}{\sqrt{3}}\right) \tag{18}$$

where the "non-zeroness" of the results can be seen from the fact that in these three states we will necessarily have the $|1,0\rangle|1/2,1/2\rangle$ with some Clebsh-Gordan coefficient, unrelevant for us now! The last 2 results are again for extra practice!

3. **Problem**

Find the phase shift corresponding to $l = 0$ in the case of the following spherical potential:

$$V(r) = \begin{cases} 0 & \text{if } \quad r > R \\ -V_0 & \text{if } \quad r \leq R \end{cases}$$

The time independent Schrödinger equation has the following form in coordinate representation:

$$-\frac{1}{r}\frac{d^2}{dr^2}(r\varphi) + \frac{l(l+1)}{r^2}\varphi + \frac{2m}{\hbar^2}V(r)\varphi = k^2\varphi$$

Point out that $r\varphi = \sin(kr)$ and $r\varphi = \cos(kr)$ functions satisfy the Schrödinger equation above in the case of $l = 0$! Give the low energy limit of the total cross-section!

Solution:

We can rewrite the equation as:

$$\frac{d^2}{dr^2}(r\varphi) = -k^2(r\varphi), \text{ for } r > R \tag{19}$$

$$\frac{d^2}{dr^2}(r\varphi) = -\kappa^2(r\varphi), \text{ for } r < R \tag{20}$$

with $\kappa^2 = k^2 + \frac{2mV_0}{\hbar^2} = \frac{2m(E+V_0)}{\hbar^2}$, solved by the general linear combination $a\frac{\cos(kr)}{k} + b\frac{\sin(kr)}{k}$ and $a\frac{\cos(\kappa r)}{\kappa} + b\frac{\sin(\kappa r)}{\kappa}$, where in order to relate it to the $l = 0$ special case of the general result, $rj_0(kr) = \frac{\sin(kr)}{k}$ and $rn_0(kr) = \frac{\cos(kr)}{k}$ we wrote in the denominators the wavenumbers.
Inside the ball we can only have the regular solution, which for $l = 0$ reads: $\varphi(r < R) = \frac{\sin(\kappa r)}{\kappa}$, $\kappa^2 = k^2 + \frac{2mV_0}{\hbar^2} \equiv q^2 + k^2$, $k^2 = \frac{2mE}{\hbar^2}$, while outside we can have a general superposition, $\varphi(r > R) = a\frac{\sin(kr)}{k} + b\frac{\cos(kr)}{k} \to \tan\delta_0 = b/a$, we write the boundary conditions as

$$\frac{\sin(\kappa R)}{\kappa} = a\frac{\sin(kR)}{k} + b\frac{\cos(kR)}{k}$$
$$\cos(\kappa R) = a\cos(kR) - b\sin(kR)$$

Which can be cast into a matrix equation:

$$\begin{pmatrix} \frac{\sin(kR)}{k} & \frac{\cos(kR)}{k} \\ \cos(kR) & -\sin(kR) \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \frac{\sin(\kappa R)}{\kappa} \\ \cos(\kappa R) \end{pmatrix}$$

Using the general inversion of a 2×2 matrix we have $\left(\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right)^{-1} = \frac{1}{ad-bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$ with the trivial substitutions we get that:

$$\tan\delta_0 = -\frac{\sin(kR)\cos(\kappa R)/k - \cos(kR)\sin(\kappa R)/\kappa}{\sin(kR)\sin(\kappa R)/\kappa + \cos(kR)\cos(\kappa R)/k} = \frac{k\tan(\kappa R) - \kappa\tan(kR)}{k\tan(kR)\tan(\kappa R) + \kappa}$$

Let us investigate the low energy limit, with $k \ll 1$ and $q^2 = \frac{2mV_0}{\hbar^2}$, we have for the terms, $\kappa \approx q$, $k\tan(\kappa R) \approx k\tan(qR)\,, -\kappa\tan(kR) \approx -\kappa k R\,, k\tan(kR)\tan(\kappa R) \sim k^2 \approx 0$, so in total we have

$$\tan\delta_0 \approx kR\left(\frac{1}{qR}\tan(qR) - 1\right)$$

for which the corresponding cross section, using the relation $\sin^2 x = \frac{\tan^2 x}{1+\tan^2 x}$

$$\sigma_0(k) = \frac{4\pi}{k^2}\frac{\tan^2\delta_0}{\tan^2\delta_0 + 1} \approx \frac{4\pi}{k^2}\tan^2\delta_0 = 4\pi R^2\left(\frac{1}{qR}\tan(qR) - 1\right)^2$$

4. **Problem** **25 pont**

Consider a one dimensional particle with q charge initially in a harmonic oscillator ground state

$$\varphi_0\left(x\right) = \frac{1}{\sqrt{x_0\sqrt{\pi}}}e^{-\frac{x^2}{2x_0^2}}\,,$$

at time $t = 0$ we switch on an $\mathcal{E}$ homogenous electric field

$$H = \frac{p^2}{2m} - \mathcal{E}qx\,.$$

Determine the time-dependence of the variance of the x coordinate operator!

Solution

$$x(t) = e^{\frac{i}{\hbar}Ht}xe^{-\frac{i}{\hbar}Ht}$$

$$[H,x] = \frac{\hbar}{i}\frac{p}{m}, [H,[H,x]] = \frac{\hbar}{i}[H,\frac{p}{m}] = -\frac{\hbar}{i}\frac{q\mathcal{E}}{m}[x,p] = \left(\frac{\hbar}{i}\right)^2\frac{q\mathcal{E}}{m}$$

Applying the Haussdorff expansion:

$$x(t) = x + \frac{p}{m}t + \frac{q\mathcal{E}}{m}t^2\,,$$

from which it follows that

$$x^2(t) = e^{\frac{i}{\hbar}Ht}x^2e^{-\frac{i}{\hbar}Ht} = e^{\frac{i}{\hbar}Ht}xe^{-\frac{i}{\hbar}Ht}e^{\frac{i}{\hbar}Ht}xe^{-\frac{i}{\hbar}Ht} = x(t)x(t)$$

$$\Downarrow$$

$$x^2(t) = x^2 + \frac{p^2}{m^2}t^2 + \frac{q^2\mathcal{E}^2}{m^2}t^4 + \frac{xp+px}{m}t - 2x\frac{q\mathcal{E}}{m}t^2 - 2p\frac{q\mathcal{E}}{m^2}t^3$$

Exploiting the fact that φ_0 is an eigenstate of a linear harmonic oscillator

$$\langle x\left(t\right)\rangle = \langle\varphi_0|x(t)|\varphi_0\rangle = \frac{q\mathcal{E}}{m}t^2$$

and

$$\left\langle x^2\right\rangle = \frac{x_0^2}{2}$$

$$\left\langle p^2\right\rangle = \frac{p_0^2}{2}\quad\left(p_0 = \frac{\hbar}{x_0}\right)$$

$$xp + px \sim \left(a + a^+\right)\left(a - a^+\right) + \left(a - a^+\right)\left(a + a^+\right)$$

$$\left(a + a^+\right)\left(a - a^+\right) = a^2 - a^{+2} + a^+a - aa^+$$
$$\left(a - a^+\right)\left(a + a^+\right) = a^2 - a^{+2} - a^+a + aa^+$$

$$xp + px \sim a^2 - a^{+2}$$

$$\Downarrow$$

$$\langle \varphi_0 | xp + px | \varphi_0 \rangle = 0$$

From where

$$\langle x^2 (t) \rangle = \langle \varphi_0 | x^2(t) | \varphi_0 \rangle = \frac{x_0^2}{2} + \frac{p_0^2}{2m^2} t^2 + \frac{q^2 \mathcal{E}^2}{m^2} t^4$$

implying for the variance

$$\langle x^2 \rangle - \langle x \rangle^2 = \frac{x_0^2}{2} + \frac{p_0^2}{2m^2} t^2$$