Problem 1. [C-T Exercise 13-1] Consider a one-dimensional harmonic oscillator of mass m, angular frequency ω_0 and charge q. Let $|\varphi_n\rangle$ and $E_n = (n+\frac{1}{2})\hbar\omega_0$ be the eigenstates and eigenvalues of its Hamiltonian $\hat{H}_0$.
For $t<0$, the oscillator is in the ground state $|\varphi_0\rangle$. At $t=0$, it is subjected to an electric field "pulse" of duration τ. The corresponding perturbation can be written $\hat{W}(t) = \begin{cases} -q\mathscr{E}\hat{x}, & 0\leq t\leq \tau, \\ 0, & t<0, t>\tau \end{cases}$ Here $\mathscr{E}$ is the field amplitude and $\hat{x}$ and $\hat{x}$ is the position observerble. Let $\mathscr{P}(0n)$ be the probability of finding the oscillator in the state $|\varphi_n\rangle$ after the pulse.

(a) Calculate $\mathscr{P}_{01}$ by using first-order time-dependent perturbation theory. How does $\mathscr{P}_{01}$ vary with τ, for fixed ω_0?

(b) Show that, to obtain $\mathscr{P}_{02}$, the time-dependent perturbation theory calculation must be pursued at least to second order. Calculate $\mathscr{P}_{02}$ to this perturbation order.

Solution:

(a) Using first-order time-dependent perturbation theory, the probability of finding the oscillator in the state $|\varphi_n\rangle$ after the pulse is

$$\mathscr{P}_{01} = \frac{1}{\hbar^2}\left|\int_0^t dt' e^{i\omega_{10}t'}W_{10}(t')\right|^2 \tag{1}$$

where the upper bound of the integral $t>\tau$, the Bohr angular frequency between the initial state $|\varphi_0\rangle$ and the final state $|\varphi_1\rangle$ is

$$\omega_{10} = \frac{E_1 - E_0}{\hbar} = \omega_0 \tag{2}$$

and the matrix element of the perturbation is

$$\begin{aligned}
W_{10}(t) =& \langle\varphi_1|\hat{W}(t)|\varphi_0\rangle = \begin{cases} -q\mathscr{E}\langle\varphi_1|\hat{x}|\varphi_0\rangle, & 0\leq t\leq\tau \\ 0, & t<0, t>\tau \end{cases} \\
=& \begin{cases} -q\mathscr{E}\sqrt{\frac{\hbar}{2m\omega_0}}\langle\varphi_1|(\hat{a}+\hat{a}^\dagger)|\varphi_0\rangle, & 0\leq t\leq\tau \\ 0, & t<0, t>\tau \end{cases} \\
=& \begin{cases} -q\mathscr{E}\sqrt{\frac{\hbar}{2m\omega_0}}\langle\varphi_1|\varphi_1\rangle, & 0\leq t\leq\tau \\ 0, & t<0, t>\tau \end{cases} \\
=& \begin{cases} -q\mathscr{E}\sqrt{\frac{\hbar}{2m\omega_0}}, & 0\leq t\leq\tau \\ 0, & t<0, t>\tau \end{cases}
\end{aligned} \tag{3}$$

Therefore,

$$\begin{aligned}
\mathscr{P}_{01} =& \frac{1}{\hbar^2}\left|-q\mathscr{E}\sqrt{\frac{\hbar}{2m\omega_0}}\int_0^\tau dt' e^{i\omega_0 t}\right|^2 \\
=& \frac{1}{\hbar^2}\left|q\mathscr{E}\sqrt{\frac{\hbar}{2m\omega_0}}\frac{e^{i\omega_0\tau}-1}{\omega_0}\right|^2 \\
=& \frac{1}{\hbar^2}\left|q\mathscr{E}\sqrt{\frac{\hbar}{2m\omega_0}}\frac{e^{i\omega_0\tau/2}-e^{-i\omega_0\tau/2}}{\omega_0}\right|^2 \\
=& \frac{1}{\hbar^2}\left|q\mathscr{E}\sqrt{\frac{\hbar}{2m\omega_0}}\frac{2i\sin(\omega_0 t/2)}{\omega_0}\right|^2 \\
=& \frac{2q^2\mathscr{E}^2}{m\hbar\omega_0^3}\sin^2\left(\frac{\omega_0 t}{2}\right) = \frac{q^2\mathscr{E}^2}{m\hbar\omega_0^3}(1-\cos\omega_0 t)
\end{aligned} \tag{4}$$

$\mathscr{P}_{01}$ oscillates with τ, for fixed ω_0. When $t = \frac{2m\pi}{\omega_0}$, $(m = 0, 1, 2, \cdots)$, $\mathscr{P}_{01}$ reaches its maximum $\mathscr{P}_{01} = \frac{q\mathscr{E}}{m\hbar\omega^3}$, and when $t = \frac{(2m+1)\pi}{\omega_0}$, $(m = 0, 1, 2, \cdots)$, $\mathscr{P}_{01}$ reaches its minimum $\mathscr{P}_{01} = 0$.

(b) We first calculate $\mathscr{P}_{02}$ to first order.

$$\mathscr{P}_{02} = \frac{1}{\hbar^2}\left|\int_0^t dt' e^{i\omega_{20}t'} W_{20}(t')\right|^2 \tag{5}$$

where the matrix element of $\hat{W}$ is

$$\begin{aligned}W_{20}(t) =& \langle\varphi_2|\hat{W}(t)|\varphi_0\rangle\\ =&\begin{cases} -q\mathscr{E}\sqrt{\frac{\hbar}{2m\omega_0}}\langle\varphi_2|\varphi_1\rangle, & 0 \leq t \leq \tau\\ 0, & t < 0, t > \tau\end{cases}\\ =&0\end{aligned} \tag{6}$$

Therefore, to first order,

$$\mathscr{P}_{02} = 0 \tag{7}$$

which means that

$$b_2(t) = b_2^{(0)}(t) + \lambda b_2^{(1)}(t) = 0 \tag{8}$$

and

$$b_2^{(1)}(t) = 0 \tag{9}$$

We must pursue the time-dependent perturbation theory calculation to the second order.

$$b_2(t) = b_2^{(0)}(t) + \lambda b_2^{(1)}(t) + \lambda^2 b_2^{(2)}(t) \tag{10}$$

The perturbation equation in the 2nd order is

$$i\hbar\frac{d}{dt}b_2^{(2)}(t) = \sum_k e^{i\omega_{nk}t} W_{2k}(t) b_k^{(1)}(t) \tag{11}$$

$$\Longrightarrow i\hbar\frac{d}{dt}b_2^{(2)} = e^{i\omega_{20}t} W_{21}(t) b_1^{(1)}(t) \tag{12}$$

$$\Longrightarrow b_2^{(2)}(t) = b_2^{(2)}(0) + \frac{1}{i\hbar}\int_0^t e^{i\omega_{21}} W_{21} b_1^{(1)}(t) = \frac{1}{i\hbar}\int_0^t e^{i\omega_{21}t} W_{21}(t) b_1^{(1)}(t) \tag{13}$$

The probability of finding the oscillator in the state $|\varphi_2\rangle$ is

$$\mathscr{P}_{20}(t) = |b_2(t)|^2 = |b_2^{(2)}(t)|^2 = \frac{1}{\hbar^2}\left|\int_0^t dt' e^{i\omega_{21}t'} W_{21}(t') b_1^{(1)}(t')\right|^2 \tag{14}$$

where $t > \tau$, the Bohr angular frequency between the state $|\varphi_2\rangle$ and $|\varphi_1\rangle$ is

$$\omega_{21} = \frac{E_2 - E_1}{\hbar} = \omega_0 \tag{15}$$

the element of $\hat{W}$ is

$$\begin{aligned}\mathscr{P}_{21} =& \langle\varphi_2|\hat{W}(t)|\varphi_1\rangle\\ =&\begin{cases} -q\mathscr{E}\sqrt{\frac{\hbar}{2m\omega_0}}\langle\varphi_2|\sqrt{2}|\varphi_2\rangle, & 0 \leq t \leq \tau\\ 0, & t < 0, t > \tau\end{cases}\\ =&\begin{cases} -q\mathscr{E}\sqrt{\frac{\hbar}{m\omega_0}}, & 0 \leq t \leq \tau\\ 0, & t < 0, t > \tau\end{cases}\end{aligned} \tag{16}$$

and

$$\mathscr{P}_{01}(t)=|b_1^{(1)}(t)|^2=\frac{q^2\mathscr{E}^2}{2m\hbar\omega_0^3}\left|e^{i\omega_0 t}-1\right|^2\Longrightarrow b_1^{(1)}(t)=q\mathscr{E}\sqrt{\frac{1}{2m\hbar\omega_0^3}}(e^{i\omega_0 t}-1)e^{i\phi_1} \tag{17}$$

Therefore,

$$\begin{aligned}\mathscr{P}_{20}=&\frac{1}{\hbar^2}\left|-q\mathscr{E}\sqrt{\frac{\hbar}{m\omega_0}}q\mathscr{E}\sqrt{\frac{1}{2m\hbar\omega_0^3}}\int_0^\tau dt'e^{i\omega_0 t'}(e^{i\omega_0 t'}-1)\right|^2\\=&\frac{1}{\hbar^2}\left|\frac{q^2\mathscr{E}^2}{\sqrt{2}m\omega_0^2}\int_0^\tau dt'e^{2i\omega_0 t'}-e^{i\omega_0 t'}\right|^2\\=&\frac{1}{\hbar^2}\left|\frac{q^2\mathscr{E}^2}{\sqrt{2}m\omega_0^2}\left(\frac{e^{2i\omega_0\tau}-1}{2\omega_0}-\frac{e^{i\omega_0\tau}-1}{\omega_0}\right)\right|^2\\=&\frac{q^2\mathscr{E}^2}{2m^2\hbar^2\omega_0^6}\left|\frac{e^{2i\omega\tau}}{2}-e^{i\omega_0\tau}+\frac{1}{2}\right|^2\end{aligned} \tag{18}$$

□

Problem 2. [C-T Exercise 13-2] Consider two spin 1/2's, $\hat{\vec{S}}_1$ and $\hat{\vec{S}}_2$, coupled by an interaction of the form $a(t)\hat{\vec{S}}_1\cdot\hat{\vec{S}}_2$; $a(t)$ is a function of time which approaches zero when $|t|$ approaches infinity, and takes on non-negligible values (on the order of a_0) only inside an interval, whose width is of the order of τ, about $t=0$.

(a) At $t=-\infty$, the system is in the state $|+-\rangle$ (an eigenstate of $\hat{\vec{S}}_1$ and $\hat{\vec{S}}_2$ with the eigenvalues $\hbar/2$ and $-\hbar/2$). Calculate, without approximations, the state of the system at $t=+\infty$. Show that the probability $\mathscr{P}(+-\to-+)$ of finding, at $t=+\infty$, the system in the state $|-+\rangle$ depends only on the integral $\int_{-\infty}^{+\infty}dt\,a(t)$.

(b) Calculate $\mathscr{P}(+-\to-+)$ by using first-order time-dependent perturbation theory. Discuss the validity conditions for such an approximation by comparing the results obtained with those of the preceding question.

(c) Now assume that the two spins are also interacting with a static magnetic field $\vec{B}_0$ parallel to Oz. The corresponding Zeeman Hamiltonian can be written $\hat{H}_0=-B_0(\gamma_1\hat{S}_{1z}+\gamma\hat{S}_{2z})$, where γ_1 and γ_2 are the gyromagnetic ratios of the two spins, assumed to be different.
Assume that $a(t)=a_0e^{-t^2/\tau^2}$. Calculate $\mathscr{P}(+-\to-+)$ by first-order time-dependent perturbation theory. With fixed a_0 and τ, discuss the variation of $\mathscr{P}(+-\to-+)$ with respect to B_0.

Solution:

(a) The initial state of the system can also be written as in the basis of $\{sm\}$

$$|\psi(t=-\infty)\rangle=|+-\rangle=\frac{1}{\sqrt{2}}[|00\rangle+|10\rangle] \tag{19}$$

The coupling energy of the system in the state represented by the eigenvector $|sm\rangle$ in the basis $\{|sm\rangle\}$ is

$$\begin{aligned}\hat{W}(t)|sm\rangle=&a(t)\hat{\vec{S}}_1\cdot\hat{\vec{S}}_2|sm\rangle\\=&\frac{1}{2}a(t)(\hat{s}^2-\hat{s}_1^2-\hat{s}_2^2)|sm\rangle\\=&\frac{1}{2}a(t)\hbar^2[s(s+1)-\frac{3}{2}]|sm\rangle\end{aligned} \tag{20}$$

$$\Longrightarrow E_{sm}=\frac{1}{2}a(t)\hbar^2[s(s+1)-\frac{3}{2}] \tag{21}$$

so $|sm\rangle$ is also an eigenvector of $W(t)$.

The Schrödinger equation is

$$i\hbar\frac{d|\psi\rangle}{dt}=\hat{W}|\psi\rangle \tag{22}$$

$$i\hbar\frac{d}{dt}\sum_{s,m}c_{sm}(t)|sm\rangle=\hat{W}(t)\sum_{sm}c_{sm}(t)|sm\rangle \tag{23}$$

$$\Longrightarrow i\hbar\frac{d}{dt}\sum_{s,m}c_{sm}(t)|sm\rangle=\frac{1}{2}a(t)\hbar^2\sum_{s,m}[s(s+1)-\frac{3}{2}]c_{sm}|sm\rangle \tag{24}$$

$$\Longrightarrow i\hbar\frac{d}{dt}c_{sm}(t)=\frac{1}{2}a(t)\hbar^2[s(s+1)-\frac{3}{2}]c_{sm} \tag{25}$$

$$\Longrightarrow\frac{\dot{c}_{sm}}{c_{sm}}=\frac{-i\hbar}{2}[s(s+1)-\frac{3}{2}]a(t) \tag{26}$$

$$\Longrightarrow(\ln c_{sm})|_{-\infty}^{\infty}=\frac{-i\hbar}{2}[s(s+1)-\frac{3}{2}]\int_{-\infty}^{\infty}dta(t) \tag{27}$$

$$c_{sm}(+\infty)=c_{sm}(-\infty)e^{\frac{-i\hbar}{2}[s(s+1)-\frac{3}{2}]\int_{-\infty}^{+\infty}dta(t)} \tag{28}$$

Given the initial state as (19), the final state of the system is

$$|\psi(t=+\infty)\rangle=\frac{1}{\sqrt{2}}(e^{\frac{3i\hbar}{4}}|00\rangle+e^{\frac{-i\hbar}{4}}|10\rangle)e^{\int_{-\infty}^{+\infty}dta(t)} \tag{29}$$

Since $|+-\rangle$ can be written as in the basis of $\{|sm\rangle\}$

$$|+-\rangle=\frac{1}{\sqrt{2}}[|10\rangle-|00\rangle] \tag{30}$$

The probability of finding, at $t=+\infty$, the system in the state $|-+\rangle$ is

$$\begin{aligned}\mathscr{P}(+-\to-+)=&\mathscr{P}(|\psi(+\infty)\rangle=|-+\rangle)=|\langle-+|\psi(+\infty)\rangle|^2\\=&\left|\frac{1}{\sqrt{2}}(-\langle00|+\langle10|)\frac{1}{\sqrt{2}}(e^{\frac{3i\hbar}{4}\int_{-\infty}^{+\infty}dta(a)}|00\rangle+e^{\frac{-i\hbar}{4}\int_{-\infty}^{+\infty}dta(t)}|10\rangle)\right|^2\\=&\frac{1}{4}\left|(-e^{\frac{3i\hbar}{4}\int_{-\infty}^{+\infty}dta(t)}+e^{\frac{-i\hbar}{4}\int_{-\infty}^{+\infty}dta(t)})\right|^2\end{aligned} \tag{31}$$

which depends only on the integral $\int_{-\infty}^{+\infty}dta(t)$.

(b) Using first-order time-dependent perturbation theory, the probability of finding, at $t=+\infty$, the system in the state $|-+\rangle$ is

$$\mathscr{P}(+-\to-+)=\frac{1}{\hbar^2}\left|\int_{-\infty}^{+\infty}dte^{i\omega_{fi}t}W_{fi}(t)\right|^2 \tag{32}$$

where the Bohr angular frequency between the initial state and the state $|-+\rangle$

$$\omega_{fi}=\frac{E_f-E_i}{\hbar}=0 \tag{33}$$

and the matrix element of $\hat{W}$ is

$$\begin{aligned}\hat{W}_{fi}(t)=&\langle-+|\hat{W}(t)|+-\rangle\\=&\frac{1}{\sqrt{2}}[-\langle00|+\langle10|]\hat{W}(t)\frac{1}{\sqrt{2}}[|00\rangle+|10\rangle]\\=&\frac{1}{4}a(t)\hbar^2[-\langle00|+\langle10|][-\frac{3}{2}|00\rangle+\frac{1}{2}|10\rangle]\\=&\frac{1}{2}\hbar^2a(t)\end{aligned} \tag{34}$$

Therefore,

$$\mathscr{P}(+- \to -+) = \frac{\hbar^2}{4}\left|\int_{-\infty}^{+\infty} dta(t)\right|^2 \tag{35}$$

Span $\mathscr{P}(+- \to -+)$ obtain from (a) about $\int_{-\infty}^{+\infty} dta(t) = 0$ and obtain the higher order terms, we can get

$$\mathscr{P}(+- \to -+) = \frac{1}{4}\left|(-e^{\frac{3i\hbar}{4}\int_{-\infty}^{+\infty} dta(t)} + e^{\frac{-i\hbar}{4}\int_{-\infty}^{+\infty} dta(t)})\right|^2 = \frac{\hbar^2}{4}\left|\int_{-\infty}^{+\infty} dta(t)\right|^2 + O\left(\left|\int_{-\infty}^{+\infty} dta(t)\right|^3\right) \tag{36}$$

which is the same as the result obtain in (b) above. Therefore, such an approximation to first order is valid when $\left|\int_{-\infty}^{+\infty} dta(t)\right|^2$

(c) In the static magnetic field, the energy of the initial state is

$$\begin{aligned}
E_{+-} =& \langle + - |\hat{H}_0| + -\rangle \\
=& \langle + - |(-B_0)(\gamma_1\hat{S}_{1z} + \gamma_2\hat{S}_{2z})| + -\rangle \\
=& - B_0\langle + - |(\gamma_1\frac{\hbar}{2} - \gamma_2\frac{\hbar}{2})| + -\rangle \\
=& - B_0(\gamma_1 - \gamma_2)\frac{\hbar}{2}
\end{aligned} \tag{37}$$

the energy of the state $|-+\rangle$ is

$$E_{-+} = \langle - + |\hat{H}_0| - +\rangle = -B_0(-\gamma_1 + \gamma_2)\frac{\hbar}{2}$$

The Bohr angular frequency between the two states above is

$$\omega_{fi} = \frac{E_{-+} - E_{+-}}{\hbar} = B_0(\gamma_1 - \gamma_2) \tag{38}$$

The matrix element of $\hat{W}(t)$ is

$$\hat{W}_{fi}(t) = \frac{1}{2}\hbar^2 a_0 e^{-t^2/\tau^2} \tag{39}$$

Therefore,

$$\begin{aligned}
\mathscr{P}(+- \to -+) =& \frac{1}{\hbar^2}\left|\int_{-\infty}^{+\infty} dte^{iB_0(\gamma_1-\gamma_2)t}\frac{1}{2}\hbar^2 a_0 e^{-t^2/\tau^2}\right|^2 \\
=& \frac{\hbar^2|a_0|^2}{4}\left|\int_{-\infty}^{+\infty} e^{-t^2/\tau^2 + iB_0(\gamma_1-\gamma_2)}\right|^2 \\
=& \frac{\hbar^2|a_0|^2}{4}\left|e^{-\left[\frac{B_0(\gamma_1-\gamma_2)\tau}{2}\right]^2}\int_{-\infty}^{+\infty} e^{-\frac{1}{\tau^2}\left[t-\frac{iB_0(\gamma_1-\gamma_2)\tau}{2}\right]^2}\right|^2 \\
=& \frac{\hbar^2|a_0|^2}{4}\left|e^{-\left[\frac{B_0(\gamma_1-\gamma_2)\tau}{2}\right]^2}\int_{-\infty}^{+\infty}\sqrt{\pi}\tau\right|^2 \\
=& \frac{\pi^2\hbar^2|a_0|^2\tau^2}{4}e^{-\frac{B_0^2(\gamma_1-\gamma_2)^2\tau^2}{2}}
\end{aligned} \tag{40}$$

$\mathscr{P}(+- \to -+)$ decreases exponentially as B_0 increases.

□

Problem 3. A particle of mass μ is scattered by the central field $V(r) = \frac{\alpha}{r^2}$ with $\alpha > 0$. Find the differential and total scattering cross section under the first-order Born approximation.

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Solution: Under the first-order Born approximation, the differential scattering cross section is

$$\begin{aligned}
\frac{d\sigma_k^{(B)(\theta,\phi)}}{d\Omega}=&\frac{\mu^2}{4\pi^2\hbar^4}\left|\int d^3re^{-i\vec{q}\cdot\vec{r}}V(\vec{r})\right|^2\\
=&\frac{\mu^2}{4\pi^2\hbar^4}\left|\int d^3re^{-i\vec{q}\cdot\vec{r}}\alpha r^{-2}\right|^2\\
=&\frac{\mu^2}{4\pi^2\hbar^4}\left|\int_0^{+\infty}dr'r'^2\int_{-1}^{+1}d(\cos\theta')\int_0^{2\pi}d\phi e^{-2ikr'\sin(\theta/2)\cos\theta'}\alpha r'^{-2}\right|^2\\
=&\frac{\mu^2}{4\pi^2\hbar^4}\left|2\pi\alpha\int_0^{+\infty}dr'\int_{-1}^{+1}d(\cos\theta')e^{-2ikr'\sin(\theta/2)\cos\theta'}\right|^2\\
=&\frac{\mu^2}{4\pi^2\hbar^4}\left|2\pi\alpha\int_0^{+\infty}dr'\frac{-2i\sin[2kr'\sin(\theta/2)]}{-2kr'\sin(\theta/2)}\right|^2\\
=&\frac{\mu^2}{4\pi^2\hbar^4}\left|\frac{2\alpha\pi}{k\sin(\theta/2)}\int_0^{+\infty}d[2kr'\sin(\theta/2)]\frac{\sin[2kr'\sin(\theta/2)]}{2kr'\sin(\theta/2)}\right|^2\\
&(\text{let }2kr'\sin(\theta/2)=\xi)\\
=&\frac{\mu^2}{4\pi^2\hbar^4}\left|\frac{2\alpha\pi}{k\sin(\theta/2)}\int_0^{+\infty}d\xi\frac{\sin\xi}{\xi}\right|^2\\
=&\frac{\mu^2}{4\pi^2\hbar^4}\left|\frac{2\alpha\pi}{k\sin(\theta/2)}\frac{\pi}{2}\right|^2\\
=&\frac{\pi^2\alpha^2\mu^2}{4\hbar^4k^2\sin^2(\theta/2)}
\end{aligned}\tag{41}$$

The total scattering cross section is

$$\begin{aligned}
\sigma_t=&\int d\Omega\frac{d\sigma(\theta,\phi)}{d\Omega}\\
=&\int_{-1}^{+1}d(\cos\theta)\int_0^{2\pi}d\phi\frac{\pi^2\alpha^2\mu^4}{4\hbar^4k^2\sin^2(\theta/2)}\\
=&\frac{2\pi^3\alpha^2\mu^4}{4\hbar^4k^2\sin^2(\theta/2)}\int_{-1}^{+1}d(\cos\theta)\frac{1}{\sin^2(\theta/2)}\\
=&\frac{2\pi^3\alpha^2\mu^4}{4\hbar^4k^2\sin^2(\theta/2)}\int_{-1}^{+1}d(\cos\theta)\frac{2}{1-\cos\theta}\\
=&\frac{2\pi^3\alpha^2\mu^4}{4\hbar^4k^2\sin^2(\theta/2)}\left[-2\ln(1-\cos\theta)\right]_{\cos\theta=-1}^{+1}\\
=&\infty
\end{aligned}\tag{42}$$

□

Problem 4. [C-T Complement C_{VIII}-3 Exercise b] Consider a central potential $V(r)$ such that $V=\begin{cases}-V_0, & r<r_0,\\ 0, & r>0.\end{cases}$ Here V_0 is a positive constant. Set $k_0=\sqrt{2\mu V_0/\hbar^2}$ with μ the mass of the particle subject to the potential. We shall confine ourselves to the study of the s wave ($l=0$).

(a) Bound states ($E<0$)]

i. Write the radial equation in the two regions $r>r_0$ and $r<r_0$, as well as the condition at the origin. Show that, if one sets $\rho=\sqrt{-2\mu E/\hbar^2}$ and $K=\sqrt{k_0^2-\rho^2}$, the function $u_0(r)$ is necessarily of the form $u_0(r)=\begin{cases}Ae^{-\rho r}, & r>r_0\\ B\sin(Kr), & r<r_0\end{cases}$

ii. Write the matching conditions at $r = R_0$. Deduce from them that the only possible values for ρ are those which satisfy the equation $\tan(Kr_0) = -K/\rho$.

iii. Discuss the equation $\tan(Kr_0) = -K/\rho$. Indicate the number of s bound states as a function of the depth of the well (for fixed r_0) and show, in particular, that there are no bound states if this depth is too small.

(b) Scattering resonances ($E > 0$)]

i. Again write the radial equation, this time setting $k = \sqrt{2\mu E/\hbar}$ and $K' = \sqrt{k_0^2 + k^2}$. Show that $u_{k,0}(r)$ is of the form $u_{k,0} = \begin{cases} A\sin(kr + \delta_0), & r > r_0, \\ B\sin(K'r), & r < r_0. \end{cases}$

ii. Choosing $A = 1$. Show, using the continuity conditions aT $r = r_0$, that the constant B and the phase shift δ_0 are given by $B^2 = k^2/[k^2 + k_0^2\cos^2(K'r_0)]$ and $\delta_0 = -kr_0 + \alpha(k)$ with $\tan\alpha(k) = (k/K')\tan(K'r_0)$.

iii. Trace the curve representing B^2 as a function of k. This curve clearly shows resonances, for which B^2 is maximum. What are the values of k associated with these resonances? What is then the value of $\alpha(k)$? Show that, if there exists such a resonance for a small energy ($kr_0 \ll 1$), the corresponding contribution of the s wave to the total cross section is practically maximal.

(c) Relation between bound states and scattering resonances
Assume that k_0r_0 is very close to $(2n+1)\pi/2$, where n is an integer, and set $k_0r_0 = (2n+1)\pi/2+\varepsilon$ with $|\varepsilon| \ll 1$.

i. Show that, if ε is positive, there exists a bound state whose binding energy $E = -\hbar^2\rho^2/2\mu$ is given by $\rho \approxeq \varepsilon k_0$.

ii. Show that if, on the other hand, ε is negative, there exists a scattering resonance at energy $E = \hbar^2k^2/2\mu$ such that $k^2 \approxeq -2k_0\varepsilon/r_0$.

iii. Deduce from this that if the depth of the well is gradually decreased (for fixed r_0), the bound state which disappears when k_0r_0 passes through an odd multiple of $\pi/2$ gives rise to a low energy scattering resonance.

Solution:

(a) i. The stationary state wave functions in the central potential can be written as

$$\varphi_{klm}(\vec{r}) = R_{kl}(r)Y_{lm}(\theta,\phi) = \frac{u_{kl}(r)}{r}Y_lm(\theta,\phi) \tag{43}$$

The general radical equation is

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)}{2\mu r^2} + V(r)\right]u_{kl}(r) = \frac{\hbar^2k^2}{2\mu}u_{kl}(r) \tag{44}$$

Confined to s wave (l=0), in the region $r > r_0$,

$$\left[\frac{d^2}{dr^2} - \rho^2\right]u_{k0}(r) = 0, \quad r > r_0 \tag{45}$$

and in the region $r < r_0$,

$$\left[\frac{d^2}{dr^2} + K^2\right]u_{k0}(r) = 0, \quad r < r_0 \tag{46}$$

The general solution to equation (45) is

$$u_{k0}(r) = A_+ e^{\rho r} + A_- e^{-\rho r}, \quad r > r_0 \tag{47}$$

Considering the boundary condition,

$$\lim_{r\to\infty}(r) \to 0 \tag{48}$$
$$\Longrightarrow A_+ = 0 \tag{49}$$

so relabel A_- as A,

$$u_{k0}(r) = Ae^{-\rho r}, \quad r > r_0 \tag{50}$$

The general solution to equation (46) is

$$u_{k0}(r) = B_+ e^{iKr} + B_- e^{-iKr}, \quad r < r_0 \tag{51}$$

Considering the condition at the origin,

$$u_{k0}(r) = 0 \Longrightarrow B_+ = -B_- = B \tag{52}$$

so

$$u_{k0}(r) = B\sin Kr, \quad r < r_0 \tag{53}$$

ii. The matching conditions at $r = r_0$ are

$$B\sin Kr_0 = Ae^{-\rho r_0} \tag{54}$$
$$BK\cos Kr_0 = -\rho Ae^{-\rho r_0} \tag{55}$$

Dividing the two equations above, we get

$$\tan Kr_0 = -\frac{K}{\rho} \tag{56}$$

iii. The number of s bound states is equal to the number of the intersection of the curve $y(K) = \tan Kr_0$ and $y(k) = -\frac{K}{\rho} = -\frac{1}{\sqrt{\frac{k_0^2}{J}-1}}$ as shown in figure 1, where $0 < K < k_0$ due to $-V < E < 0$ for bound states.

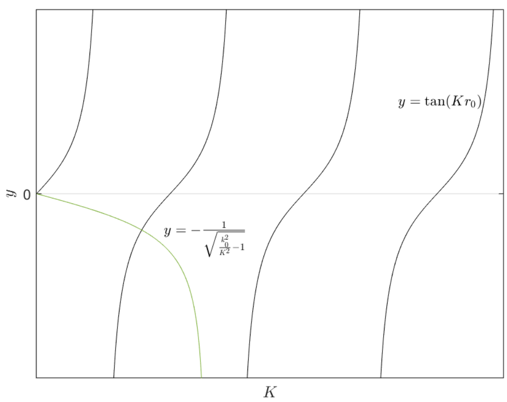

图 1: Problem 5 (a) iii.

The number of intersections of the two curves within $(0, k_0)$ is

$$n = \left\lceil \frac{k_0}{\pi/r_0} - \frac{1}{2} \right\rceil = \left\lceil \frac{\sqrt{2\mu V_0/\hbar^2}}{\pi/r_0} - \frac{1}{2} \right\rceil \tag{57}$$

If $k_0 \leq \frac{\pi}{2r_0}$, the two curves do not have any intersection within $(0, k_0)$.

(b) i. In the region $r > r_0$, the radical equation is

$$\left[\frac{d^2}{dr^2} + k^2\right] u_{k0}(r) = 0, \quad r > r_0 \tag{58}$$

In the region $r < r_0$, the radical equation is

$$\left[\frac{d^2}{dr^2} + K'^2\right] u_{k0}(r) = 0, \quad r < r_0 \tag{59}$$

The general solution to (58) is

$$u_{k0}(r) = A_+ e^{ikr} + A_- e^{-ikr}, \quad r > r_0 \tag{60}$$

The setting of scattering resonance is equivalent to a one-dimensional problem with $V(r) = \infty$ for $r < 0$, in which $|A_-|^2$ is the amplitude of the incident plane wave and $|A_+|^2$ is the amplitude of the reflected plane wave at large r. Since there is no transmission, we have

$$|A_+|^2 = |A_-|^2 \tag{61}$$

$$\Longrightarrow u_{k0}(r) = A(e^{ikr}e^{i\phi_+} + e^{-ikr}e^{i\phi_-}) = A\sin(kr + \delta_0), \quad r > r_0 \tag{62}$$

The general solution to equation (59) is

$$u_{k0} = B_+ e^{iK'r} + B_- e^{iK'r}, \quad r < r_0 \tag{63}$$

Considering the condition at origin,

$$u_{k0}(0) = 0 \tag{64}$$

we have

$$B_+ = B_- = \frac{B}{2} \tag{65}$$

so

$$u_{k0}(r) = B\sin(K'r), \quad r < r_0 \tag{66}$$

Therefore,

$$u_{k0}(r) = \begin{cases} A\sin(kr + \delta_0), & r > r_0, \\ B\sin(K'r), & r < r_0. \end{cases} \tag{67}$$

ii. The matching conditions at $r = r_0$ are

$$\sin(kr_0 + \delta_0) = B\sin(K'r_0) \tag{68}$$

$$k\cos(kr_0 + \delta_0) = BK'\cos(K'r_0) \tag{69}$$

Square the two equations above, we get

$$\sin^2(kr_0 + \delta_0) = B^2\sin^2(K'r_0) \tag{70}$$

$$\cos^2(kr_0 + \delta_0) = B^2\frac{K'^2}{k^2}\cos(K'r_0) \tag{71}$$

Add the two equations above, we get

$$1 = B^2 \left[\sin^2(K'r_0) + \frac{K'^2}{k^2}\cos^2(K'r_0)\right] \tag{72}$$

$$\Longrightarrow B^2 = \frac{1}{\left[1 - \cos^2(K'r_0) + \frac{K'^2}{k^2}\cos^2(K'r_0)\right]} \tag{73}$$

$$\Longrightarrow B^2 = \frac{k^2}{k^2 + k_0^2\cos^2(K'r_0)} \tag{74}$$

Devide the two equations at the beginning, we get

$$\tan(kr_0 + \delta_0) = \frac{k}{K'}\tan(K'r_0) \tag{75}$$

Using $\delta_0 = -kr_0 + \alpha(k)$, we get

$$\tan\alpha(k) = \frac{k}{K'}\tan(K'r_0) \tag{76}$$

iii. The minima occur at $\cos^2(K'r_0) = 0$ or

$$K'r_0 = \sqrt{k_0^2 + k^2} = \frac{(2n+1)\pi}{2r_0} \tag{77}$$

$$k = \sqrt{\left(\frac{(2n+1)\pi}{2r_0}\right)^2 - k_0^2} \tag{78}$$

where n is integer.

At these values of k, $\tan(K'r_0)$ blows up, as does $\tan\alpha(k)$, so

$$\alpha(k) = (m + \frac{1}{2})\pi \tag{79}$$

where m is integer.

The total cross section is

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \tag{80}$$

For $kr_0 \ll 1$, at resonace

$$\begin{aligned}\sin^2\delta_0 =& \sin^2(-kr_0 + \alpha(k))\\ =& \sin^2\left(-kr_0 + (m + \frac{1}{2})\pi\right)\\ =& [(-1)^m\cos kr_0]^2\\ =& \cos^2 kr_0\\ =& 1 - (kr_0)^2 + O[(kr_0)^4]\end{aligned} \tag{81}$$

Therefore, $\sin\delta_0$ is practically maximal.

(c) i. Guess $\rho \approx \varepsilon k_0$ when $k_0 r_0 = (n+\frac{1}{2})\pi + \varepsilon$ with ε positive and $\varepsilon \ll 1$,

$$\begin{aligned}\tan(Kr_0) =& \tan\sqrt{k_0^2-\rho^2}r_0\\ =& \tan\left[(1-\varepsilon^2)^{1/2}\left((n+\frac{1}{2})\pi+\varepsilon\right)\right]\\ =& \tan\left[(1-\frac{1}{2}\varepsilon^2+O(\varepsilon^4))\left((n+\frac{1}{2})\pi+\varepsilon\right)\right]\\ =& \tan\left[(n+\frac{1}{2})\pi+O(\varepsilon^2)\right]\\ =& -\cot\left[\varepsilon+O(\varepsilon^2)\right]\\ =& -\frac{\cos\left[\varepsilon+O(\varepsilon^2)\right]}{\sin\left[\varepsilon+O(\varepsilon^2)\right]}\\ =& -\frac{1-\frac{1}{2}\varepsilon^2+O(\varepsilon^3)}{\varepsilon}\\ =& -\frac{1}{\varepsilon}+\frac{1}{2}\varepsilon+O(\varepsilon^2)\end{aligned} \tag{82}$$

$$\begin{aligned}-\frac{K}{\rho} =& -\frac{\sqrt{k_0^2-\rho^2}}{\rho}\\ =& -\frac{1-\varepsilon^2}{\varepsilon}\\ =& -\frac{1-\frac{1}{2}\varepsilon^2+O(\varepsilon^3)}{\varepsilon}\\ =& -\frac{1}{\varepsilon}+\frac{1}{2}\varepsilon+O(\varepsilon^2)\end{aligned} \tag{83}$$

$$\Longrightarrow \tan(Kr_0) = -\frac{K}{\rho} \tag{84}$$

so the guess is correct.

ii. The resonance condition is

$$k^2 = \left((n+\frac{1}{2})\frac{\pi}{r_0}\right)^2 - k_0^2 \tag{85}$$

Plug $k_0 = \frac{1}{r_0}[(n+\frac{1}{2})\frac{\pi}{2}+\varepsilon]$ into the equation above, we get

$$\begin{aligned}k^2 =& \left((n+\frac{1}{2})\frac{\pi}{r_0}\right) - \frac{1}{r_0^2}\left[(n+\frac{1}{2})\pi+\varepsilon\right]^2\\ =& \left((n+\frac{1}{2})\frac{\pi}{r_0}\right)^2 - \frac{1}{r_0^2}\left((n+\frac{1}{2})\pi\right)^2 - \frac{2\varepsilon}{r_0^2}\left((n+\frac{1}{2})\pi\right) - \frac{\varepsilon^2}{r_0^2}\\ =& -\frac{2\varepsilon}{r_0^2}\left((n+\frac{1}{2})\pi\right) - \frac{\varepsilon^2}{r_0^2}\\ =& -\frac{2k_0\varepsilon}{r_0} + O(\varepsilon^2)\end{aligned}$$

iii. When the depth of the well is gradually decreased or k_0 gradually decreased and $k_0 r_0$ pass through an odd multiple of $\frac{\pi}{2}$, one of the intersections in figure 1 disappears and resonance appears in (ii) at about the same energy.

Reference: `https://phys.cst.temple.edu/~meziani/homework2s_5702_2017.pdf` □

Problem 5. [C-T Exercise 14-3] Consider the state space of an electron, spanned by the two vectors $|\varphi_{p_x}\rangle$ and $|\varphi_{p_y}\rangle$ which represent two atomic orbitals, p_x and p_y, of wave functions $\varphi_{p_x}(\vec{r})$ and $\varphi_{p_y}(\vec{r})$, $\varphi_{p_x}(\vec{r}) = xf(r) = rf(r)\sin\theta\cos\phi$, $\varphi_{p_y}(\vec{r}) = yf(r) = rf(r)\sin\theta\sin\phi$.

(a) Write, in terms of $|\varphi_{p_x}\rangle$ and $|\varphi_{p_y}\rangle$, the state $|\varphi_{p_\alpha}\rangle$ which represents the p_α orbital pointing in the direction of the xOy plane which makes an angle α with Ox.

(b) Consider two electrons whose spins are both in the $|+\rangle$ state, the eigenstate of $\hat{S}_z$ of eigenvalue $+\hbar/2$. Write the normalized state vector $|\psi\rangle$ which represents the system of two electrons, one of which is in the state $|\varphi_{p_x}\rangle$ and the other in the state $|\varphi_{p_y}\rangle$.

(c) Same question, with one of the electrons in the state $|\varphi_{p_\alpha}\rangle$ and the other one in the state $|\varphi_{p_\beta}\rangle$, where α and β are two arbitrary angles. Show that the state vector $|\psi\rangle$ obtained is the same.

(d) The system is in the state $|\psi\rangle$ of question (b). Calculate the probability density $\mathscr{P}(r,\theta,\phi;r',\theta',\phi)$ of finding one electron at (r,θ,ϕ) and the other one at (r',θ',ϕ'). Show that the electronic density $\rho(r,\theta,\phi)$ [the probability density of finding any electron at (r,θ,ϕ)] is symmetrical wich respect to revolution about the Oz axis. Determine the probability density of having $\phi-\phi'=\phi_0$, where ϕ_0 is given. Discuss the variation of this probability density with respect to ϕ_0.

Solution:

(a) The state which represents the p_α orbital pointing in the direction of the xOy plane which makes an angle α with Ox is

$$|\varphi_{p_\alpha}\rangle=\cos\alpha|\varphi_{p_x}\rangle+\sin\alpha|\varphi_{p_y}\rangle \tag{86}$$

(b) The state vector which represents the system of two electrons, one of which is in the state $|\varphi_{p_x}\rangle$ and the other in the state $|\varphi_{p_y}\rangle$ is

$$|\psi_{12}\rangle=\frac{1}{\sqrt{2}}\begin{vmatrix}|\psi_1\rangle & |\psi_1\rangle\\ |\psi_2\rangle & |\psi_2\rangle\end{vmatrix}=\frac{1}{\sqrt{2}}(|\psi_1\rangle|\psi_2\rangle-|\psi_2\rangle|\psi_1\rangle) \tag{87}$$

where

$$|\psi_1\rangle=|\varphi_{p_x}\rangle\otimes|+\rangle \tag{88}$$
$$|\psi_2\rangle=|\varphi_{p_y}\rangle\otimes|+\rangle \tag{89}$$

Therefore,

$$|\psi_{12}\rangle=\frac{1}{\sqrt{2}}(|\varphi_{p_x}\varphi_{p_y}\rangle-|\varphi_{p_y}\varphi_{p_x}\rangle)|++\rangle \tag{90}$$

(c) Let

$$|\psi_1\rangle=(\cos\alpha|\varphi_{p_x}\rangle+\sin\alpha|\varphi_{p_y}\rangle)\otimes|+\rangle \tag{91}$$
$$|\psi_2\rangle=(\cos\beta|\varphi_{p_x}\rangle+\sin\beta|\varphi_{p_y}\rangle) \tag{92}$$

For simplicity, write

$$|+\rangle=\alpha(s_i) \tag{93}$$

where $i=1$ or 2 depending on the particle.

$$\begin{aligned}\psi_1(\vec{r}_1,s_1)\psi_2(\vec{r}_2,s_2)=&\alpha(s_1)\alpha(s_2)(\cos\alpha\varphi_{p_x}(\vec{r}_1)+\sin\alpha\varphi_{p_y}(\vec{r}_1))(\cos\beta\varphi_{p_x}(\vec{r}_2)+\sin\beta\varphi_{p_y}(\vec{r}_2))\\ =&\alpha(s_1)\alpha(s_2)[\cos\alpha\cos\beta\varphi_{p_x}(\vec{r}_1)\varphi_{p_x}(\vec{r}_2)+\cos\alpha\sin\beta\varphi_{p_x}(\vec{r}_1)\varphi_{p_y}(\vec{r}_2)\\ &+\sin\alpha\cos\beta\varphi_{p_y}(\vec{r}_1)\varphi_{p_x}(\vec{r}_2)+\sin\alpha\sin\beta\varphi_{p_y}(\vec{r}_1)\varphi_{p_y}(\vec{r}_2)]\end{aligned} \tag{94}$$

and

$$\begin{aligned}\psi_2(\vec{r}_1,s_1)\psi_1(\vec{r}_2,s_2)=&\alpha(s_1)\alpha(s_2)(\cos\beta\varphi_{p_x}(\vec{r}_1)+\sin\beta\varphi_{p_y}(\vec{r}_1))(\cos\alpha\varphi_{p_x}(\vec{r}_2)+\sin\alpha\varphi_{p_y}(\vec{r}_2))\\=&\alpha(s_1)\alpha(s_2)[\cos\beta\cos\alpha\varphi_{p_x}(\vec{r}_1)\varphi_{p_x}(\vec{r}_2)+\cos\beta\sin\alpha\varphi_{p_x}(\vec{r}_1)\varphi_{p_y}(\vec{r}_2)\\&+\sin\beta\cos\alpha\varphi_{p_y}(\vec{r}_1)\varphi_{p_x}(\vec{r}_2)+\sin\beta\sin\alpha\varphi_{p_y}(\vec{r}_1)\varphi_{p_y}(\vec{r}_2)]\end{aligned}\tag{95}$$

Therefore,

$$\begin{aligned}|\psi_{12}\rangle=&\frac{1}{\sqrt{2}}(|\psi_1\rangle|\psi_2\rangle-|\psi_2\rangle|\psi_1\rangle)|++\rangle\\=&\frac{1}{\sqrt{2}}[\varphi_{p_x}(\vec{r}_1)\varphi_{p_y}(\vec{r}_2)(\cos\alpha\sin\beta-\cos\beta\sin\alpha)+\varphi_{p_y}(\vec{r}_1)\varphi_{p_x}(\vec{r}_2)(\sin\alpha\cos\beta-\cos\alpha\sin\beta)]|++\rangle\\=&\frac{1}{\sqrt{2}}[\varphi_{p_x}(\vec{r}_1)\varphi_{p_y}(\vec{r}_2)-\varphi_{p_y}(\vec{r}_1)\varphi_{p_x}(\vec{r}_2)]|++\rangle\sin(\beta-\alpha)\end{aligned}$$

After normalization,

$$|\psi_{12}\rangle=\frac{1}{\sqrt{2}}[\varphi_{p_x}(\vec{r}_1)\varphi_{p_y}(\vec{r}_2)-\varphi_{p_y}(\vec{r}_1)\varphi_{p_x}(\vec{r}_2)]|++\rangle\tag{96}$$

which is the same as the result obtained in (b).

(d) Since we are not to observe the spin, the spin part of the state vector can be hidden.

$$|\psi_{12}\rangle=\frac{1}{\sqrt{2}}[\varphi_{p_x}(\vec{r}_1)\varphi_{p_y}(\vec{r}_2)-\varphi_{p_y}(\vec{r}_1)\varphi_{p_x}(\vec{r}_2)]\tag{97}$$

$$\Longrightarrow\psi_{12}(r,\theta,\phi;r',\theta',\phi')=\frac{1}{\sqrt{2}}rr'f(r)f(r')\sin\theta\sin\theta'(\cos\phi\sin\phi'-\sin\phi\cos\phi')\tag{98}$$

$$=\frac{1}{\sqrt{2}}rr'f(r)f(r')\sin\theta\sin\theta'\sin(\phi'-\phi)\tag{99}$$

The probability density of finding one electron at (r,θ,ϕ) and the other one at (r',θ',ϕ') is

$$\begin{aligned}\mathscr{P}(r,\theta,\phi;r',\theta',\phi')=&\langle\psi_{12}|\psi_{12}\rangle\\=&|\psi_{12}(r,\theta,\phi;r',\theta',\phi')|^2r^2r'^2\sin\theta\sin\theta'\\=&\frac{1}{2}r^4r'^4|f(r)|^2|f(r')|^2\sin^4\theta\sin^4\theta'\sin^2(\phi'-\phi)\\=&F(r,\theta;r',\theta')\sin^2(\phi'-\phi)\end{aligned}\tag{100}$$

The electron density is

$$\rho(r,\theta,\phi)=\int_0^{+\infty}r^2dr\int_0^\pi\sin\theta'd\theta'\int_0^{2\pi}d\phi'\mathscr{P}(r,\theta,\phi;r',\theta',\phi')\tag{101}$$

When we rotate with respect to z axis

$$\phi\to\phi+\phi_0\tag{102}$$

$$\phi'\to\phi'+\phi_0\tag{103}$$

The probability density becomes

$$\begin{aligned}\mathscr{P}(r,\theta,\phi+\phi_0;r',\theta',\phi'+\phi_0)=&F(r,\theta;r',\theta')\sin^2[(\phi'+\phi_0)-(\phi+\phi_0)]\\=&F(r,\theta;r',\theta')\sin^2(\phi'-\phi)\\=&\mathscr{P}(r,\theta,\phi;r',\theta',\phi')\end{aligned}\tag{104}$$

The probability density is symmetrical to revolution about the Oz axis, so the electron density is also symmetrical to revolution about the Oz.
When $\phi - \phi' = \phi_0$, the this probability density is

$$\mathscr{P}(r,\theta,\phi;r',\theta',\phi') = F(r,\theta;r',\theta')\sin^2(\phi_0) \propto \sin^2(\phi_0) \tag{105}$$

□