Quantum Mechanics: Fall 2020
Midterm Exam: Brief Solutions

NOTE: Problems start on page 2. Bold symbols are 3-component vectors.

Some useful facts: You can use them directly.

- 1D harmonic oscillator: $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}x^2$.
  Here $\hat{x}$ is position operator, $\hat{p}$ is momentum operator, $[\hat{x},\hat{p}] = \mathbb{i}\hbar$, and in position representation $\hat{p} = -\mathbb{i}\hbar\frac{\partial}{\partial x}$. Define $\hat{a}_\mp = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} \pm \mathbb{i}\frac{1}{m\omega}\hat{p}) = \sqrt{\frac{m\omega}{2\hbar}}(x \pm \frac{\hbar}{m\omega}\frac{\partial}{\partial x})$. Then $[\hat{a}_-,\hat{a}_+] = 1$ and $\hat{H} = \hbar\omega\,(\hat{a}_+\hat{a}_- + \frac{1}{2})$. It has a unique ground state $|\psi_0\rangle$ with $\hat{a}_-|\psi_0\rangle = 0$, and excited states $|\psi_n\rangle \equiv \frac{1}{\sqrt{n!}}(\hat{a}_+)^n|\psi_0\rangle$ with energy $E_n = (n+\frac{1}{2})\hbar\omega$. The ground state wavefunction is $\psi_0(x) = (\frac{m\omega}{\pi\hbar})^{1/4}\exp(-\frac{m\omega}{2\hbar}x^2)$.

- $\int_{-\infty}^{+\infty} e^{-x^2/a}\mathrm{d}x = \sqrt{\pi a}$, for $a > 0$. Applying $\frac{\partial}{\partial a}$ can produce $\int_{-\infty}^{+\infty} x^{2n}e^{-x^2/a}\mathrm{d}x$.

- Central potential problem: $\hat{H} = \frac{1}{2m}\hat{\boldsymbol{p}}^2 + V(r)$.
  Here $\hat{\boldsymbol{p}}$ is the 3D momentum $-\mathbb{i}\hbar\frac{\partial}{\partial \boldsymbol{r}}$, and $r = |\boldsymbol{r}|$ is the radius. Under polar coordinates (r,θ,ϕ), the eigenfunctions are generally $\psi_{E,\ell,m} = \frac{u(r)}{r}\cdot Y_\ell^m(\theta,\phi)$, where $Y_\ell^m(\theta,\phi)$ is the spherical harmonics, and $u(r)$ satisfies $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]\cdot u = E\cdot u$. Here $\ell = 0, 1, \ldots$ is the angular momentum quantum number; $m = -\ell, -\ell+1, \ldots, \ell$ is the "magnetic quantum number"; E is the energy eigenvalue.

  - The spherical harmonics are orthonormal, and are eigenfunctions of $\hat{\boldsymbol{L}}^2$ and $\hat{L}_z$. $Y_0^0 = \frac{1}{\sqrt{4\pi}}$, $Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$, $Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm\mathbb{i}\phi}$, $\ldots$.

- Generic angular momentum: $[\hat{J}_x,\hat{J}_y] = \mathbb{i}\hbar\hat{J}_z$, $[\hat{J}_y,\hat{J}_z] = \mathbb{i}\hbar\hat{J}_x$, $[\hat{J}_z,\hat{J}_x] = \mathbb{i}\hbar\hat{J}_y$.
  For eigenstate $|j,m\rangle$ of $\hat{\boldsymbol{J}}^2$ and $\hat{J}_z$, $\hat{\boldsymbol{J}}^2|j,m\rangle = j(j+1)\hbar^2|j,m\rangle$, $\hat{J}_z|j,m\rangle = m\hbar|j,m\rangle$, and $(\hat{J}_x \pm \mathbb{i}\hat{J}_y)|j,m\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}|j,m\pm 1\rangle$.
  Here $2j$ is non-negative integer, $m = -j, -j+1, \ldots, j$.

  - Orbital angular momentum: $\hat{\boldsymbol{L}} \equiv \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}$.
  - Spin-1/2: basis states $|\uparrow\rangle$ and $|\downarrow\rangle$. Under this basis, $\hat{S}_a = \frac{\hbar}{2}\sigma_a$, where $\sigma_{x,y,z}$ are Pauli matrices, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -\mathbb{i} \\ \mathbb{i} & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. $\sigma_a\sigma_b = \delta_{ab}\mathbb{1}_{2\times 2} + \mathbb{i}\sum_c \epsilon_{abc}\sigma_c$.
    Generic wavefunction under this basis is $\begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}$, which means $\psi_\uparrow|\uparrow\rangle + \psi_\downarrow|\downarrow\rangle$.
  - $\sum_a \epsilon_{abc}\epsilon_{adf} = \delta_{bd}\delta_{cf} - \delta_{bf}\delta_{cd}$.

Problem 1. (35 points) Consider the 1D harmonic oscillator (see page 1) under a constant force, $\hat{H}' = \hat{H} - f \cdot \hat{x} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{x}^2}{2} - f \cdot \hat{x}$, where f is a real constant.

(a) (5pts) *Write down the ground state wave function $\psi_0'(x)$ of $\hat{H}'$.* [Hint: you can directly read off the result; but for later questions, it's better to find new ladder operators $\hat{a}'_\pm = \hat{a}_\pm + (\text{constant})$, such that $[\hat{a}'_-, \hat{a}'_+] = 1$, $\hat{H}' = \hbar\omega \cdot \hat{a}'_+ \hat{a}'_- + (\text{constant})$, then $\hat{a}'_- \psi_0' = 0$.]

(b) (10pts) Measure the original Hamiltonian $\hat{H}$ under $\psi_0'(x)$. *What are the possible measurement results and their probabilities?* [Hint: ψ_0' is actually a "coherent state"].

(c) (10pts) Let the initial state be $\psi(x, t = 0) = \psi_0'(x)$. Evolve it by $\hat{H}$ (not $\hat{H}'$), namely $\mathrm{i}\hbar \frac{\partial}{\partial t} \psi(x, t) = \hat{H}\psi(x, t)$. *Solve the explicit expression of $\psi(x, t)$.* [Hint: $\psi(x, t)$ would still be a coherent state.]

(d) (10pts) *Evaluate expectation values $\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$, $\langle \hat{x}^2 \rangle$, $\langle \hat{p}^2 \rangle$, under the state $\psi(x, t)$ defined in (c). Check that the uncertainty relation $\sigma_{\hat{x}}^2 \cdot \sigma_{\hat{p}}^2 \geq \frac{\hbar^2}{4}$ is satisfied.*

Solution: this is essentially the same as homework Problem 3.35.

(a) $\hat{H}' = -\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega^2}{2}(x - \frac{f}{m\omega^2})^2 - \frac{f^2}{2m\omega^2}$.

Define $x' = x - \frac{f}{m\omega^2}$, then $\hat{p}' = -\mathrm{i}\hbar\partial_{x'} = \hat{p}$, $\hat{H}' = -\frac{\hbar^2}{2m}\partial_{x'}^2 + \frac{m\omega^2}{2}x'^2 - \frac{f^2}{2m\omega^2}$.

Therefore the eigenstates are $\psi_n(x') = \psi_n(x - \frac{f}{m\omega^2})$ with energy $E_n' = E_n - \frac{f^2}{2m\omega^2} = \hbar\omega \cdot (n + \frac{1}{2}) - \frac{f^2}{2m\omega^2}$.

The ground state is $\psi_0'(x) = \psi_0(x - \frac{f}{m\omega^2}) = (\frac{m\omega}{\pi\hbar})^{1/4} \exp[-\frac{m\omega}{2\hbar}(x - \frac{f}{m\omega^2})^2]$.

Define $\hat{a}'_\pm = \sqrt{\frac{m\omega}{2\hbar}}(x' \mp \mathrm{i}\frac{\hat{p}'}{m\omega}) = \hat{a}_\pm - \sqrt{\frac{m\omega}{2\hbar}}\frac{f}{m\omega^2}$.

Then $[\hat{a}'_-, \hat{a}'_+] = 1$, $\hat{H}' = \hbar\omega\hat{a}'_+\hat{a}'_- + \frac{1}{2}\hbar\omega - \frac{f^2}{2m\omega^2}$, $\hat{a}'_-\psi_0' = 0$.

(b) $\hat{a}'_-\psi_0' = 0$, namely $\hat{a}_-\psi_0' = \sqrt{\frac{m\omega}{2\hbar}}\frac{f}{m\omega^2} \cdot \psi_0'$, for notation simplicity, define $\alpha = \sqrt{\frac{m\omega}{2\hbar}}\frac{f}{m\omega^2}$, then this is the same as homework Problem 3.35.

ψ_0' is a coherent state, and can be expanded in terms of $\hat{H}$ eigenstates as [Problem 3.35(c)], $\psi_0'(x) = \sum_{n=0}^{\infty} c_n\psi_n(x) = \sum_{n=0}^{\infty} e^{-|\alpha|^2/2}\frac{\alpha^n}{\sqrt{n!}}\psi_n(x)$.

Measuring $\hat{H}$ can get result $E_n = \hbar\omega(n + \frac{1}{2})$ with probability $|c_n|^2 = e^{-|\alpha|^2}\frac{|\alpha|^{2n}}{n!}$ (Poisson distribution).

(c) $\psi(x,t) = \sum_{n=0}^{\infty} e^{-\mathrm{i}E_n t/\hbar} c_n \psi_n(x) = e^{-\mathrm{i}\omega t/2} \sum_{n=0}^{\infty} e^{-|\alpha|^2/2} \frac{(\alpha e^{-\mathrm{i}\omega t})^n}{\sqrt{n!}} \psi_n(t)$.

So except for the overall phase factor $e^{-\mathrm{i}\omega t/2}$, this is still a coherent state, with α replaced by $\alpha e^{-\mathrm{i}\omega t}$ [Problem 3.35(e)].

Therefore $\hat{a}_- \psi(x,t) = \alpha e^{-\mathrm{i}\omega t} \cdot \psi(x,t)$.

$\sqrt{\frac{m\omega}{2\hbar}}(x + \frac{\hbar}{m\omega}\partial_x)\psi(x,t) = \sqrt{\frac{m\omega}{2\hbar}} \frac{f}{m\omega^2} e^{-\mathrm{i}\omega t}\psi(x,t)$.

$-\frac{m\omega}{\hbar}(x - \frac{f}{m\omega^2}e^{-\mathrm{i}\omega t})\mathrm{d}x = \frac{\mathrm{d}\psi}{\psi} = \mathrm{d}(\log\psi)$.

Then $\psi \propto \exp(-\frac{m\omega}{2\hbar}x^2 + \frac{f}{\hbar\omega}e^{-\mathrm{i}\omega t}x) \propto \exp\{-\frac{m\omega}{2\hbar}[x - \frac{f}{m\omega^2}\cos(\omega t)]^2\}\exp[-\mathrm{i}\frac{f}{\hbar\omega}\sin(\omega t)x]$.

Normalize it and put back the overall $e^{-\mathrm{i}\omega t/2}$ factor,

$\psi(x,t) = e^{-\mathrm{i}\omega t/2}(\frac{m\omega}{\pi\hbar})^{1/4}\exp\{-\frac{m\omega}{2\hbar}[x - \frac{f}{m\omega^2}\cos(\omega t)]^2\}\exp[-\mathrm{i}\frac{f}{\hbar\omega}\sin(\omega t)x]$.

As consistency check, when $f = 0$, this is $\psi_0(x,t)$.

(d) this is the same as Problem 3.35(a)

Use $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_- + \hat{a}_+)$, $\hat{p} = \frac{m\omega}{\mathrm{i}}\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_- - \hat{a}_+)$, $\hat{a}_-|\psi(x,t)\rangle = \alpha e^{-\mathrm{i}\omega t}\cdot|\psi(x,t)\rangle$, and therefore $\langle\psi(x,t)|\hat{a}_+ = \langle\psi(x,t)|\cdot\alpha^* e^{\mathrm{i}\omega t}$.

$\langle\hat{x}\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\alpha e^{-\mathrm{i}\omega t} + \alpha^* e^{+\mathrm{i}\omega t}) = \frac{f}{m\omega^2}\cos(\omega t)$.

$\langle\hat{p}\rangle = \frac{m\omega}{\mathrm{i}}\sqrt{\frac{\hbar}{2m\omega}}(\alpha e^{-\mathrm{i}\omega t} - \alpha^* e^{+\mathrm{i}\omega t}) = -\frac{f}{\omega}\sin(\omega t)$.

$\langle\hat{x}^2\rangle = \frac{\hbar}{2m\omega}\cdot\langle\hat{a}_-^2 + \hat{a}_+^2 + 2\hat{a}_+\hat{a}_- + 1\rangle = \frac{\hbar}{2m\omega}\{[\frac{f}{m\omega^2}\cos(\omega t)]^2 + 1\}$

$\langle\hat{p}^2\rangle = (m\omega)^2\frac{\hbar}{2m\omega}\cdot\langle-\hat{a}_-^2 - \hat{a}_+^2 + 2\hat{a}_+\hat{a}_- + 1\rangle = \frac{\hbar m\omega}{2}\{[\frac{f}{\omega}\sin(\omega t)]^2 + 1\}$

Therefore $\sigma_x^2 = \frac{\hbar}{2m\omega}$, $\sigma_p^2 = \frac{\hbar m\omega}{2}$, and $\sigma_x^2\sigma_p^2 = \frac{\hbar^2}{4}$, satisfies the minimal uncertainty relation.

Problem 2. (20 points) Consider the electron in hydrogen atom with Hamiltonian $\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{\mathrm{e}^2}{4\pi\epsilon_0}\frac{1}{r}$. Note that electron is spin-1/2 particle, so should be described by spinor wave function $\begin{pmatrix}\psi_\uparrow(\boldsymbol{r})\\ \psi_\downarrow(\boldsymbol{r})\end{pmatrix}$. Restrict the orbital wave functions within the $n = 2$ energy level, namely $\psi_{\uparrow,\downarrow}$ are linear combinations of normalized eigenstates $\psi_{2\ell m} = R_{2l}(r)Y_\ell^m(\theta,\phi)$ of spinless hydrogen atom problem. Define the total angular momentum operators $\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$.

(a) (5pts) *Show explicitly that* $[\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{L}}^2] = 0$, $[\hat{\boldsymbol{J}}^2, \hat{J}_z] = 0$, $[\hat{\boldsymbol{L}}^2, \hat{J}_z] = 0$.

(b) (5pts) *Within this restricted Hilbert space, what are the possible combinations of eigenvalues of* $\hat{\boldsymbol{J}}^2$ *and* $\hat{\boldsymbol{L}}^2$ *and* $\hat{J}_z$.

(c) (10pts) *Solve the normalized spinor wave functions* ψ_{j,ℓ,m_j} *of eigenstates of*

$\hat{\boldsymbol{J}}^2 = j(j+1)\hbar^2$ *and* $\hat{\boldsymbol{L}}^2 = \ell(\ell+1)\hbar$ *and* $\hat{J}_z = m_j\hbar$ *within this restricted Hilbert space, in terms of* $\psi_{2\ell m}$. NOTE: you don't need explicit formula of $\psi_{2\ell m}$.

Solution: this problem is related to homework Problem 4.36(b) and 4.19(c).

(a) the calculation is related to homework Problem 4.19(c),

First show that $[\hat{J}_a, \hat{L}_b] = \mathrm{i}\hbar \sum_c \epsilon_{abc}\hat{L}_c$, then $[\hat{J}_a, \hat{\boldsymbol{L}}^2] = [\hat{J}_a, \sum_b \hat{L}_b^2] = \mathrm{i}\hbar \sum_{b,c}(\epsilon_{abc}\hat{L}_c\hat{L}_b + \epsilon_{abc}\hat{L}_b\hat{L}_c) = \mathrm{i}\hbar \sum_{b,c} \hat{L}_b\hat{L}_c(\epsilon_{acb} + \epsilon_{abc}) = 0$, then $[\hat{\boldsymbol{J}}^2, \hat{\boldsymbol{L}}^2] = [\sum_a \hat{J}_a^2, \hat{\boldsymbol{L}}^2] = 0$.

Similarly, $[\hat{J}_a, \hat{J}_b] = \mathrm{i}\hbar \sum_c \epsilon_{abc}\hat{J}_c$ leads to $[\hat{J}_a, \hat{\boldsymbol{J}}^2] = 0$.

(b)(c) The nontrivial C.-G. coefficients used here are also used in Problem 4.36(b).

For $n = 2$ energy level of hydrogen atom, ℓ can be 0 or 1.

When $\ell = 1$, j can be $\frac{3}{2}$ or $\frac{1}{2}$; when $\ell = 0$, j must be $\frac{1}{2}$. $m_j = -j, \ldots, j$.

The results are

(j, ℓ, m_j)	$\hat{\boldsymbol{J}}^2$	$\hat{\boldsymbol{L}}^2$	$\hat{J}_z$	ψ_{j,ℓ,m_j}
$(\frac{3}{2}, 1, \frac{3}{2})$	$\frac{15}{4}\hbar^2$	$2\hbar^2$	$\frac{3}{2}\hbar$	$\begin{pmatrix} \psi_{2,\ell=1,m=1} \\ 0 \end{pmatrix}$
$(\frac{3}{2}, 1, \frac{1}{2})$	$\frac{15}{4}\hbar^2$	$2\hbar^2$	$\frac{1}{2}\hbar$	$\frac{1}{\sqrt{3}}\begin{pmatrix} \sqrt{2}\psi_{2,\ell=1,m=0} \\ \psi_{2,\ell=1,m=1} \end{pmatrix}$
$(\frac{3}{2}, 1, -\frac{1}{2})$	$\frac{15}{4}\hbar^2$	$2\hbar^2$	$-\frac{1}{2}\hbar$	$\frac{1}{\sqrt{3}}\begin{pmatrix} \psi_{2,\ell=1,m=-1} \\ \sqrt{2}\psi_{2,\ell=1,m=0} \end{pmatrix}$
$(\frac{3}{2}, 1, -\frac{3}{2})$	$\frac{15}{4}\hbar^2$	$2\hbar^2$	$-\frac{3}{2}\hbar$	$\begin{pmatrix} 0 \\ \psi_{2,\ell=1,m=-1} \end{pmatrix}$
$(\frac{1}{2}, 1, \frac{1}{2})$	$\frac{3}{4}\hbar^2$	$2\hbar^2$	$\frac{1}{2}\hbar$	$\frac{1}{\sqrt{3}}\begin{pmatrix} \psi_{2,\ell=1,m=0} \\ -\sqrt{2}\psi_{2,\ell=1,m=1} \end{pmatrix}$
$(\frac{1}{2}, 1, -\frac{1}{2})$	$\frac{3}{4}\hbar^2$	$2\hbar^2$	$-\frac{1}{2}\hbar$	$\frac{1}{\sqrt{3}}\begin{pmatrix} \sqrt{2}\psi_{2,\ell=1,m=-1} \\ -\psi_{2,\ell=1,m=0} \end{pmatrix}$
$(\frac{1}{2}, 0, \frac{1}{2})$	$\frac{3}{4}\hbar^2$	0	$\frac{1}{2}\hbar$	$\begin{pmatrix} \psi_{2,\ell=0,m=0} \\ 0 \end{pmatrix}$
$(\frac{1}{2}, 0, -\frac{1}{2})$	$\frac{3}{4}\hbar^2$	0	$-\frac{1}{2}\hbar$	$\begin{pmatrix} 0 \\ \psi_{2,\ell=0,m=0} \end{pmatrix}$

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up to overall phase factor of ψ_{j,ℓ,m_j} for the same j, ℓ.

Problem 3. (30 points) Consider two spin-1/2 moments $\hat{\boldsymbol{S}}_1$ and $\hat{\boldsymbol{S}}_2$, satisfying $[\hat{S}_{i,a}, \hat{S}_{j,b}] = \delta_{i,j}\mathbb{i}\hbar \sum_c \epsilon_{abc}\hat{S}_{i,c}$, for $i,j = 1,2$ and $a,b,c = x,y,z$. The basis for the entire system can be chosen as tensor products of S_z-basis $|S_1 = \frac{1}{2}, S_{1z}\rangle|S_2 = \frac{1}{2}, S_{2z}\rangle$, with $S_{1z}, S_{2z} = \pm\frac{1}{2}$. Denote them as $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ hereafter.

(a) (10pts) Consider the Hamiltonian $\hat{H} = \frac{J}{\hbar^2}\cdot(\hat{\boldsymbol{S}}_1\cdot\hat{\boldsymbol{S}}_2 - \frac{\hbar^2}{4}) - \frac{B}{\hbar}\cdot(\hat{S}_{1,x} + \hat{S}_{2,x})$. Here J, B are real constants. *Solve the eigenvalues and eigenstates (in terms of the S_z-basis) of $\hat{H}$.* [Hint: the J-term is related to total spin square $\hat{\boldsymbol{S}}^2$ where $\hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2$]

(b) (5pts) Let the initial state be $|\psi(t=0)\rangle = |\uparrow\downarrow\rangle$, evolve it under $\hat{H}$, namely $\mathbb{i}\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$. *Solve $|\psi(t)\rangle$ in terms of S_z-basis.*

(c) (5pts**) Define "vector chirality operators" $\hat{\boldsymbol{\chi}} = \hat{\boldsymbol{S}}_1 \times \hat{\boldsymbol{S}}_2$, here '$\times$' means vector cross product. *Compute the commutators $[\hat{H}, \hat{\chi}_a]$ for $a = x,y,z$, the results should be polynomials of $\hat{S}_{i,a}$ of at most degree 2.* [Hint: cyclic permutation symmetry of indices x,y,z can be used]

(d) (10pts**) *Compute the expectation values of $\hat{\boldsymbol{\chi}}$ under $|\psi(t)\rangle$ in (b).*

Solution:

(a) you can view $\hat{H}$ as a 4×4 matrix under the S_z-basis: $\hat{S}_{1,a} = \frac{\hbar}{2}\sigma_a \otimes \sigma_0$, $\hat{S}_{2,a} = \frac{\hbar}{2}\sigma_0 \otimes \sigma_a$, then $\hat{H} = -\frac{1}{2}\begin{pmatrix} 0 & B & B & 0 \\ B & J & -J & B \\ B & -J & J & B \\ 0 & B & B & 0 \end{pmatrix}$, and try to diagonalize it by brute-force (by some symmetry consideration, this can be reduced to a 2×2 problem).

Or rewrite $\hat{H} = \frac{J}{2\hbar^2}\hat{\boldsymbol{S}}^2 - J - \frac{B}{\hbar}\hat{S}_x$, where $\hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2$ is the total spin operator. Total spin quantum number S can be 1 or 0. Then the eigenvalues of $\hat{H}$ are

$\frac{J}{2\hbar^2}\cdot 1\cdot(1+1)\hbar^2 - J - \frac{B}{\hbar}\cdot m\hbar = -m\cdot B$, for $|S=1, S_x = m\rangle$ state, $m = -1, 0, 1$;

and $\frac{J}{2\hbar^2}\cdot 0\cdot(0+1)\hbar^2 - J - \frac{B}{\hbar}\cdot 0\hbar = -J$ for $|S=0, S_x=0\rangle$ state.

To get these states in terms of S_z-basis, use the cyclic permutation symmetry of indices x,y,z, then

$|S=1, S_x=1\rangle = |S_1 = \frac{1}{2}, S_{1,x} = \frac{1}{2}\rangle|S_2 = \frac{1}{2}, S_{2,x} = \frac{1}{2}\rangle$;

$|S=1, S_x=0\rangle$

$= \frac{1}{\sqrt{2}}(|S_1 = \frac{1}{2}, S_{1,x} = -\frac{1}{2}\rangle|S_2 = \frac{1}{2}, S_{2,x} = \frac{1}{2}\rangle + |S_1 = \frac{1}{2}, S_{1,x} = \frac{1}{2}\rangle|S_2 = \frac{1}{2}, S_{2,x} = -\frac{1}{2}\rangle)$;

$|S=1, S_x=-1\rangle = |S_1 = \frac{1}{2}, S_{1,x} = -\frac{1}{2}\rangle|S_2 = \frac{1}{2}, S_{2,x} = -\frac{1}{2}\rangle$.

$|S=0,S_x=0\rangle$
$=\frac{1}{\sqrt{2}}(|S_1=\frac{1}{2},S_{1,x}=-\frac{1}{2}\rangle|S_2=\frac{1}{2},S_{2,x}=\frac{1}{2}\rangle-|S_1=\frac{1}{2},S_{1,x}=\frac{1}{2}\rangle|S_2=\frac{1}{2},S_{2,x}=-\frac{1}{2}\rangle)$.

For a single spin-1/2,
$|S=\frac{1}{2},S_x=+\frac{1}{2}\rangle\propto\frac{1}{\sqrt{2}}(|\uparrow\rangle+|\downarrow\rangle)$, $|S=\frac{1}{2},S_x=-\frac{1}{2}\rangle\propto\frac{1}{\sqrt{2}}(|\uparrow\rangle-|\downarrow\rangle)$. Here the phase factors have not been determined, because we have not defined "ladder operators" for $\hat{S}_x$, and demanded Condon-Shortley convention for the ladder operators for $\hat{S}_x$.

The results are

S	S_x	$\hat{H}$	eigenstate
1	1	$-B$	$\frac{1}{2}(\lvert\uparrow\uparrow\rangle+\lvert\uparrow\downarrow\rangle+\lvert\downarrow\uparrow\rangle+\lvert\downarrow\downarrow\rangle)$
1	0	0	$\frac{1}{\sqrt{2}}(\lvert\uparrow\uparrow\rangle-\lvert\downarrow\downarrow\rangle)$
1	-1	$+B$	$\frac{1}{2}(\lvert\uparrow\uparrow\rangle-\lvert\uparrow\downarrow\rangle-\lvert\downarrow\uparrow\rangle+\lvert\downarrow\downarrow\rangle)$
0	0	$-J$	$\frac{1}{\sqrt{2}}(\lvert\uparrow\downarrow\rangle-\lvert\downarrow\uparrow\rangle)$

(b) $|\uparrow\downarrow\rangle=\frac{1}{2}|S=1,S_x=1\rangle-\frac{1}{2}|S=1,S_x=-1\rangle+\frac{1}{\sqrt{2}}|S=0,S_x=0\rangle$,
$|\psi(t)\rangle$
$=e^{-\mathrm{i}(-B)t/\hbar}\frac{1}{2}|S=1,S_x=1\rangle-e^{-\mathrm{i}(+B)t/\hbar}\frac{1}{2}|S=1,S_x=-1\rangle+e^{-\mathrm{i}(-J)t/\hbar}\frac{1}{\sqrt{2}}|S=0,S_x=0\rangle$
$=\frac{\mathrm{i}}{2}\sin(\frac{Bt}{\hbar})(|\uparrow\uparrow\rangle+|\downarrow\downarrow\rangle)+\frac{1}{2}[\cos(\frac{Bt}{\hbar})+e^{\mathrm{i}Jt/\hbar}]|\uparrow\downarrow\rangle+\frac{1}{2}[\cos(\frac{Bt}{\hbar})-e^{\mathrm{i}Jt/\hbar}]|\downarrow\uparrow\rangle$.

(c) $\hat{\chi}_a=\sum_{b,c}\epsilon_{abc}\hat{S}_{1,b}\hat{S}_{2,c}$.

Use $[\hat{S}_a,\hat{S}_{i,b}]=\mathrm{i}\hbar\sum_c\hat{S}_{i,c}$, $\sum_a\epsilon_{abc}\epsilon_{adf}=\delta_{bd}\delta_{cf}-\delta_{bf}\delta_{cd}$.

$[\hat{S}_a,\hat{\chi}_b]=[\hat{S}_a,\sum_{c,d}\epsilon_{bcd}\hat{S}_{1,c}\hat{S}_{2,d}]=\mathrm{i}\hbar\sum_{c,d,f}\epsilon_{bcd}(\epsilon_{acf}\hat{S}_{1,f}\hat{S}_{2,d}+\epsilon_{adf}\hat{S}_{1,c}\hat{S}_{2,f})$
$=\mathrm{i}\hbar(-\hat{S}_{1,b}\hat{S}_{2,a}+\hat{S}_{1,a}\hat{S}_{2,b})=\mathrm{i}\hbar\sum_c\epsilon_{abc}\hat{\chi}_c$.
Namely, $\hat{\boldsymbol{\chi}}$ transform as a vector under rotation generated by $\hat{\boldsymbol{S}}$.

For spin-1/2, $\hat{S}_{i,a}\hat{S}_{i,b}=\frac{\hbar^2}{4}\delta_{ab}+\mathrm{i}\frac{\hbar}{2}\sum_c\epsilon_{abc}\hat{S}_c$ (see page 1, about Pauli matrices).

$[\hat{\boldsymbol{S}}_1\cdot\hat{\boldsymbol{S}}_2,\hat{\chi}_a]=\sum_{b,c,d}\epsilon_{acd}(\hat{S}_{1,b}\hat{S}_{2,b}\hat{S}_{1,c}\hat{S}_{2,d}-\hat{S}_{1,c}\hat{S}_{2,d}\hat{S}_{1,b}\hat{S}_{2,b})$
$=\sum_{b,c,d}\epsilon_{acd}(\frac{\hbar^2}{4}\delta_{bc}[\hat{S}_{2,b},\hat{S}_{2,d}]+\mathrm{i}\frac{\hbar}{2}\sum_f\epsilon_{bcf}\hat{S}_{1,f}\{\hat{S}_{2,b},\hat{S}_{2,d}\})$
$=\sum_{b,c,d,f}\epsilon_{acd}(\frac{\hbar^2}{4}\delta_{bc}\mathrm{i}\hbar\epsilon_{bdf}\hat{S}_{2,f}+\mathrm{i}\frac{\hbar}{2}\epsilon_{bcf}\hat{S}_{1,f}\frac{\hbar^2}{2}\delta_{bd})=\mathrm{i}\frac{\hbar^3}{2}(\hat{S}_{2,a}-\hat{S}_{1,a})$.

Finally, $[\hat{H},\hat{\chi}_x]=\mathrm{i}\frac{\hbar J}{2}(\hat{S}_{2,x}-\hat{S}_{1,x})$, $[\hat{H},\hat{\chi}_y]=\mathrm{i}\frac{\hbar J}{2}(\hat{S}_{2,y}-\hat{S}_{1,y})-\mathrm{i}B\hat{\chi}_z$,
$[\hat{H},\hat{\chi}_z]=\mathrm{i}\frac{\hbar J}{2}(\hat{S}_{2,z}-\hat{S}_{1,z})+\mathrm{i}B\hat{\chi}_y$.

You can also compute the commutators $[\hat{S}_{1,b}\hat{S}_{2,b},\hat{\chi}_a]$ and use the cyclic permutation symmetry, so only $[\hat{S}_{1,x}\hat{S}_{2,x},\hat{\chi}_z]$, $[\hat{S}_{1,y}\hat{S}_{2,y},\hat{\chi}_z]$, $[\hat{S}_{1,z}\hat{S}_{2,z},\hat{\chi}_z]$ need to be explicitly computed.

(d) directly use the result of (b), and $\hat{\chi}_x = \frac{1}{2\mathrm{i}}[(\hat{S}_{1,+} - \hat{S}_{1,-})\hat{S}_{2,z} - \hat{S}_{1,z}(\hat{S}_{2,+} - \hat{S}_{2,-})]$, $\hat{\chi}_y = \frac{1}{2}[\hat{S}_{1,z}(\hat{S}_{2,+}+\hat{S}_{2,-})-(\hat{S}_{1,+}+\hat{S}_{1,-})\hat{S}_{2,z}]$, $\hat{\chi}_z = \frac{1}{2\mathrm{i}}[\hat{S}_{1,-}\hat{S}_{2,+}-\hat{S}_{1,+}\hat{S}_{2,-}]$, compute one-by-one the expectation values of these "non-branching terms" (each term acting on one S_z-basis will produce just one S_z-basis).

$\hat{S}_{1,+}\hat{S}_{2,z}|\psi(t)\rangle = \frac{\hbar^2}{2}\{-\frac{\mathrm{i}}{2}\sin(\frac{Bt}{\hbar})|\uparrow\downarrow\rangle + \frac{1}{2}[\cos(\frac{Bt}{\hbar}) - e^{\mathrm{i}Jt/\hbar}]|\uparrow\uparrow\rangle\}$, then
$\langle\psi(t)|\hat{S}_{1,+}\hat{S}_{2,z}|\psi(t)\rangle = \frac{\hbar^2}{8}\{-\mathrm{i}\sin(\frac{Bt}{\hbar})[\cos(\frac{Bt}{\hbar}) - e^{\mathrm{i}Jt/\hbar}] + [\cos(\frac{Bt}{\hbar}) + e^{-\mathrm{i}Jt/\hbar}](-\mathrm{i}\sin(\frac{Bt}{\hbar})\}$
$= \frac{\hbar^2}{4}[-\mathrm{i}\sin(\frac{Bt}{\hbar})\cos(\frac{Bt}{\hbar}) - \sin(\frac{Bt}{\hbar})\sin(\frac{Jt}{\hbar})]$,

$\langle\psi(t)|\hat{S}_{1,-}\hat{S}_{2,z}|\psi(t)\rangle = (\langle\psi(t)|\hat{S}_{1,+}\hat{S}_{2,z}|\psi(t)\rangle)^* = \frac{\hbar^2}{4}[+\mathrm{i}\sin(\frac{Bt}{\hbar})\cos(\frac{Bt}{\hbar}) - \sin(\frac{Bt}{\hbar})\sin(\frac{Jt}{\hbar})]$.

$\hat{S}_{1,z}\hat{S}_{2,+}|\psi(t)\rangle = \frac{\hbar^2}{2}\{-\frac{\mathrm{i}}{2}\sin(\frac{Bt}{\hbar})|\downarrow\uparrow\rangle + \frac{1}{2}[\cos(\frac{Bt}{\hbar}) + e^{\mathrm{i}Jt/\hbar}]|\uparrow\uparrow\rangle\}$, then
$\langle\psi(t)|\hat{S}_{1,z}\hat{S}_{2,+}|\psi(t)\rangle = \frac{\hbar^2}{8}\{-\mathrm{i}\sin(\frac{Bt}{\hbar})[\cos(\frac{Bt}{\hbar}) + e^{\mathrm{i}Jt/\hbar}] + [\cos(\frac{Bt}{\hbar}) - e^{-\mathrm{i}Jt/\hbar}](-\mathrm{i}\sin(\frac{Bt}{\hbar})\}$
$= \frac{\hbar^2}{4}[-\mathrm{i}\sin(\frac{Bt}{\hbar})\cos(\frac{Bt}{\hbar}) + \sin(\frac{Bt}{\hbar})\sin(\frac{Jt}{\hbar})]$,

$\langle\psi(t)|\hat{S}_{1,z}\hat{S}_{2,-}|\psi(t)\rangle = (\langle\psi(t)|\hat{S}_{1,z}\hat{S}_{2,+}|\psi(t)\rangle)^* = \frac{\hbar^2}{4}[+\mathrm{i}\sin(\frac{Bt}{\hbar})\cos(\frac{Bt}{\hbar}) + \sin(\frac{Bt}{\hbar})\sin(\frac{Jt}{\hbar})]$.

$\hat{S}_{1,-}\hat{S}_{2,+}|\psi(t)\rangle = \hbar^2 \cdot \frac{1}{2}[\cos(\frac{Bt}{\hbar}) + e^{\mathrm{i}Jt/\hbar}]|\downarrow\uparrow\rangle$, then
$\langle\psi(t)|\hat{S}_{1,-}\hat{S}_{2,+}|\psi(t)\rangle = \frac{\hbar^2}{4}[\cos(\frac{Bt}{\hbar}) - e^{-\mathrm{i}Jt/\hbar}][\cos(\frac{Bt}{\hbar}) + e^{\mathrm{i}Jt/\hbar}]$
$= \frac{\hbar^2}{4}\{[\cos(\frac{Bt}{\hbar}) + \mathrm{i}\sin(\frac{Jt}{\hbar})]^2 - \cos^2(\frac{Jt}{\hbar})\}$.

$\hat{S}_{1,+}\hat{S}_{2,-}|\psi(t)\rangle = (\hat{S}_{1,-}\hat{S}_{2,+}|\psi(t)\rangle)^* = \frac{\hbar^2}{4}\{[\cos(\frac{Bt}{\hbar}) - \mathrm{i}\sin(\frac{Jt}{\hbar})]^2 - \cos^2(\frac{Jt}{\hbar})\}$

Finally, we have
$\langle\hat{\chi}_x\rangle = 0$, $\langle\hat{\chi}_y\rangle = \frac{\hbar^2}{2}\sin(\frac{Bt}{\hbar})\sin(\frac{Jt}{\hbar})$, $\langle\hat{\chi}_z\rangle = \frac{\hbar^2}{2}\cos(\frac{Bt}{\hbar})\sin(\frac{Jt}{\hbar})$.

(Not required) You may want to use the Heisenberg equations of motion, $\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{O}\rangle = \frac{\mathrm{i}}{\hbar}\langle[\hat{H},\hat{O}]\rangle$. However we need the equations of motion for "staggered moment" operators $\hat{\boldsymbol{M}} \equiv \hat{\boldsymbol{S}}_2 - \hat{\boldsymbol{S}}_1$, to get a closed set of differential equations.

$[\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2, \hat{M}_a] = -2\mathrm{i}\hbar \cdot \hat{\chi}_a$ (textbook Problem 4.37).

$[\hat{S}_b, \hat{M}_a] = \sum_c \mathrm{i}\hbar\epsilon_{bac}\hat{M}_c$. $\hat{\boldsymbol{M}}$ transform as a vector under rotation generated by $\hat{\boldsymbol{S}}$.

Then $[\hat{H}, \hat{M}_x] = -2\mathrm{i}\frac{J}{\hbar}\hat{\chi}_x$, $[\hat{H}, \hat{M}_y] = -2\mathrm{i}\frac{J}{\hbar}\hat{\chi}_y - \mathrm{i}B\hat{M}_z$, $[\hat{H}, \hat{M}_z] = -2\mathrm{i}\frac{J}{\hbar}\hat{\chi}_z + \mathrm{i}B\hat{M}_y$.

The equations of motion are

$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\chi}_x\rangle = -\frac{J}{2}\langle\hat{M}_x\rangle$,

$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\chi}_y\rangle = -\frac{J}{2}\langle\hat{M}_y\rangle + \frac{B}{\hbar}\langle\chi_z\rangle$,

$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\chi}_z\rangle = -\frac{J}{2}\langle\hat{M}_z\rangle - \frac{B}{\hbar}\langle\chi_y\rangle$,

$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{M}_x\rangle = 2\frac{J}{\hbar^2}\langle\hat{\chi}_x\rangle$,

$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{M}_y\rangle = 2\frac{J}{\hbar^2}\langle\hat{\chi}_y\rangle + \frac{B}{\hbar}\langle\hat{M}_z\rangle$,

$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{M}_z\rangle = 2\frac{J}{\hbar^2}\langle\hat{\chi}_z\rangle - \frac{B}{\hbar}\langle\hat{M}_y\rangle$.

With the initial condition, $\langle\hat{\chi}_x\rangle = \langle\hat{\chi}_y\rangle = \langle\hat{\chi}_z\rangle = 0$, $\langle\hat{M}_x\rangle = \langle\hat{M}_y\rangle = 0$, $\langle\hat{M}_z\rangle = -\hbar$, at $t = 0$.

Define $\boldsymbol{V}_\pm = \langle\hat{\boldsymbol{\chi}}\rangle \pm \mathbb{i}\frac{\hbar}{2}\langle\hat{\boldsymbol{M}}\rangle$, then

$\frac{\mathrm{d}}{\mathrm{d}t}V_{\pm,x} = \pm\mathbb{i}\frac{J}{\hbar}V_{\pm,x}$, so $V_{\pm,x}(t) = e^{\pm\mathbb{i}Jt/\hbar}V_{\pm,x}(0) = 0$, so $\langle\hat{\chi}_x\rangle = (V_{+,x} + V_{-,x})/2 = 0$;

$\frac{\mathrm{d}}{\mathrm{d}t}V_{\pm,y} = \pm\mathbb{i}\frac{J}{\hbar}V_{\pm,y} + \frac{B}{\hbar}V_{\pm,z}$,

$\frac{\mathrm{d}}{\mathrm{d}t}V_{\pm,z} = \pm\mathbb{i}\frac{J}{\hbar}V_{\pm,z} - \frac{B}{\hbar}V_{\pm,y}$.

Define $V_{\sigma,\pm} = V_{\sigma,y} \pm \mathbb{i}V_{\sigma,z}$ where $\sigma = \pm$; then $\frac{\mathrm{d}}{\mathrm{d}t}V_{\sigma,\pm} = (\sigma\mathbb{i}\frac{J}{\hbar} \mp \mathbb{i}\frac{B}{\hbar})V_{\sigma,\pm}$.

$V_{+,+}(t) = e^{\mathbb{i}(J-B)t/\hbar}V_{+,+}(0) = e^{\mathbb{i}(J-B)t/\hbar}(\frac{\hbar^2}{2})$,

$V_{+,-}(t) = e^{\mathbb{i}(J+B)t/\hbar}V_{+,-}(0) = -e^{\mathbb{i}(J+B)t/\hbar}(\frac{\hbar^2}{2})$,

$V_{-,+}(t) = e^{\mathbb{i}(-J+B)t/\hbar}V_{-,+}(0) = -e^{\mathbb{i}(-J+B)t/\hbar}(\frac{\hbar^2}{2})$,

$V_{-,-}(t) = e^{\mathbb{i}(-J-B)t/\hbar}V_{-,-}(0) = e^{\mathbb{i}(-J-B)t/\hbar}(\frac{\hbar^2}{2})$.

Then $\langle\chi_y\rangle = (V_{+,+} + V_{+,-} + V_{-,+} + V_{-,-})/4 = \frac{\hbar^2}{2}\sin(\frac{Jt}{2})\sin(\frac{Bt}{2})$,

$\langle\chi_y\rangle = (V_{+,+} - V_{+,-} + V_{-,+} - V_{-,-})/(4\mathbb{i}) = \frac{\hbar^2}{2}\sin(\frac{Jt}{2})\cos(\frac{Bt}{2})$.

Problem 4. (15 points) Consider the harmonic oscillator with an additional δ-function potential, $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}}{2} - \alpha\cdot\delta(x)$, where α is a positive constant.

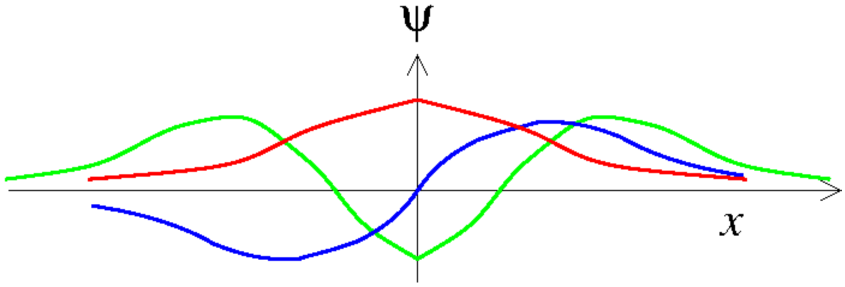
(a) (6pts) *Draw qualitatively the wave functions for the ground state, 1st excited state, and 2nd excited state.*

(b) (6pts) For the stationary Schrödinger equation $\hat{H}\psi = E\psi$, define $\xi = \sqrt{\frac{m\omega}{\hbar}}x$, $K = \frac{2E}{\hbar\omega}$, $\beta = \frac{2\alpha}{\hbar\omega}\sqrt{\frac{m\omega}{\hbar}}$. Then $\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\psi = [\xi^2 - \beta\cdot\delta(\xi) - K]\cdot\psi$. Assume $\psi(\xi) = h(\xi)\cdot e^{-\xi^2/2}$, then $\frac{\mathrm{d}^2h}{\mathrm{d}\xi^2} - 2\xi\frac{\mathrm{d}h}{\mathrm{d}\xi} + [K - 1 + \beta\cdot\delta(\xi)]\cdot h = 0$. Consider the ground state in (a), assume $h(\xi) = \sum_{j=0}^{\infty} a_j\xi^j$ for $\xi \geq 0$. *Derive the recursion relation for a_j, derive the boundary condition at $\xi = 0$ in terms of a_j.*

(c) (3pts***) The recursion relation for a_j in (b) is actually the same as the original harmonic oscillator. But the ground state energy is not the original eigenvalues of harmonic oscillator without the δ-potential, therefore the series for h will not be truncated to finite order. *How can this reconcile with the requirement that ψ should be normalizable?*

Solution:

(a) Schematic picture of the ground state, 1st excited state, and 2nd excited state.



The ground state is even, nodeless, has a cusp at $x = 0$.

The 1st excited state is odd, has one node at $x = 0$, is smooth everywhere.

The 2nd excited state is even, has two nodes, has a cusp at $x = 0$.

(b) The recursion relation is the same as the original Harmonic oscillator (textbook equation [2.81]), because the differential equation in $x > 0$ region is exactly the same as the harmonic oscillator, $a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)} a_j$.

The boundary condition at $x = 0$ should be $\partial_\xi \psi|_{\xi=-0}^{+0} = -\beta\psi(0)$.

Note that the ground state is an even function, then $h(\xi) = h(|\xi|) = \sum_{j=0}^{\infty} a_j |\xi|^j$.

$\partial_\xi \psi|_{\xi=-0}^{+0} = \partial_\xi h|_{\xi=-0}^{+0} = 2a_1$, $\psi(0) = a_0$.

So the boundary condition for even eigenstates is $a_1 = -\frac{\beta}{2} a_0$.

(c) For the ground state energy E_0' with the δ-potential, the original stationary Schrödinger equation $[-\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega^2}{2}x^2]\psi = E_0'\psi$ have two solutions (related to certain “hypergeometric functions”), one even function [the even j terms in (b)] and one odd function [the odd j terms in (b)], both solutions are asymptotically $\sim \exp(+\xi^2/2)$.

But by making a proper linear combination [“parabolic cylinder function” $D_{\frac{K-1}{2}}(\sqrt{2}\xi)$] of these two solutions, we can cancel the divergence as $\xi \to +\infty$. This linear combination would diverge as $\exp(+\xi^2/2)$ when $\xi \to -\infty$, but we are only using it for $\xi \geq 0$ region.