**Problem 1.** A particle is initially in the the ground state of an infinite one-dimensional potential box with walls at $x = 0$ and $x = L$. During the time interval $0 \le t \le \infty$, the particle is subject to a perturbation $V(t) = x^2 e^{-t/\tau}$, where $\tau$ is a time constant. Calculate, to first order in perturbation theory, the probability of finding the particle in its first excited state as a result of this perturbation.

**Solution.** The wave functions and energy eigenstates for a particle in an infinite one-dimensional box are given by Eq. (A.2.4) in Sakurai:

$$\psi_E(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \qquad E = \frac{\hbar^2 n^2 \pi^2}{2mL^2},$$

where $n = 1, 2, 3, \ldots$ Equation (5.6.19) gives the general expression for the transition probability from state $i$ to state $n$, which is

$$P(i \to n) = |c_n^{(1)}(t) + c_n^{(2)}(t) + \cdots|^2.$$

We are looking for the first order contribution, $c_n^{(1)}(t)$, which may be found using Eq. (5.6.17):

$$c_n^{(1)}(t) = -\frac{i}{\hbar}\int_{t_0}^{t} \langle n|V_I(t')|t\rangle \, dt' = -\frac{i}{\hbar}\int_{t_0}^{t} e^{i\omega_{ni}t'} V_{ni}(t') \, dt' \,, \tag{1}$$

where

$$e^{i(E_n - E_i)t/\hbar} = e^{i\omega_{ni}t}$$

from Eq. (5.6.18).

Let $\psi_n$ denote the wavefunctions corresponding to the eigenstates of $H_0$ with eigenvalue $n$. We are interested in the transition probability from $i = 1$ to $n = 2$, so the relevant wavefunctions are

$$\psi_1(t) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right), \qquad \psi_2(t) = \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right),$$

and the corresponding energies are

$$E_1 = \frac{\hbar^2\pi^2}{2mL^2}, \qquad E_2 = \frac{2\hbar^2\pi^2}{mL^2}.$$

The relevant matrix element of $V(t)$ is

$$\begin{aligned}
\langle 2|V(t)|1\rangle &= \int_0^\infty \int_0^\infty \left\langle \psi_2 \middle| x' \right\rangle \left\langle x' \middle| V \middle| x'' \right\rangle \left\langle x'' \middle| \psi_1 \right\rangle dx' \, dx'' \\
&= \frac{2}{L} e^{-t/\tau} \int_0^L \int_0^L \sin\left(\frac{2\pi x'}{L}\right) x'^2 \delta(x' - x'') \sin\left(\frac{\pi x''}{L}\right) dx' \, dx'' \\
&= \frac{2}{L} e^{-t/\tau} \int_0^L \sin\left(\frac{2\pi x'}{L}\right) x'^2 \sin\left(\frac{\pi x'}{L}\right) dx' = \frac{4}{L} e^{-t/\tau} \int_0^L x'^2 \sin^2\left(\frac{\pi x'}{L}\right) \cos\left(\frac{\pi x'}{L}\right) dx' \,.
\end{aligned}$$

Let $u = \pi x'/L$. Then

$$\begin{aligned}
\langle 2|V(t)|1\rangle &= \frac{4L^2}{\pi^3} e^{-t/\tau} \int_0^\pi u^2 \sin^2 u \cos u \, du = \frac{4L^2}{\pi^3} e^{-t/\tau} \int_0^\pi u^2 (\cos u - \cos^3 u) \, du \\
&= \frac{4L^2}{\pi^3} e^{-t/\tau} \int_0^\pi u^2 \left(\cos u - \frac{3}{4}\cos u - \frac{1}{4}\cos 3u\right) du = \frac{L^2}{\pi^3} e^{-t/\tau} \int_0^\pi u^2 \left(\cos u - \cos 3u\right) du \,.
\end{aligned}$$

For the first integral, we integrate by parts twice:

$$\int_0^\pi u^2 \cos u \, du = \Big[u^2 \sin u\Big]_0^\pi - 2\int_0^\pi u \sin u \, du = 2\Big[u \cos u\Big]_0^\pi + 2\int_0^\pi \cos u \, du = -2\pi + 2\Big[\sin u\Big]_0^\pi = -2\pi.$$

For the second, let $v = 3u$. Then we again integrate by parts twice:

$$\int_0^\pi u^2 \cos 3u \, du = \frac{1}{27}\int_0^{3\pi} v^2 \cos v \, dv = \frac{1}{27}\Big[v^2 \sin v\Big]_0^{3\pi} - \frac{2}{27}\int_0^{3\pi} v \sin v \, dv = \frac{2}{27}\Big[v \cos v\Big]_0^{3\pi} + \frac{2}{27}\int_0^{3\pi} \cos v \, dv$$
$$= -\frac{2\pi}{9} + \frac{2}{27}\Big[\sin v\Big]_0^{3\pi} = -\frac{2\pi}{9}.$$

Then our matrix element is

$$\langle 2|V(t)|1\rangle = -\frac{L^2}{\pi^2} e^{-t/\tau}\frac{16\pi}{9} = -\frac{16L^2}{9\pi^2} e^{-t/\tau}.$$

Returning to (1), we may now find the first-order coefficient. First note that

$$E_2 - E_1 = \frac{3\hbar^2\pi^3}{2mL^2}.$$

Then

$$c_n^{(1)}(t) = -\frac{i}{\hbar}\int_{t_0}^t e^{i(E_2-E_1)t'/\hbar} V_{21}(t')\, dt' = \frac{i}{\hbar}\frac{16L^2}{9\pi^2}\int_0^\infty \exp\left(i\frac{3\hbar\pi^2}{2mL^2}t'\right) e^{-t'/\tau}\, dt'$$
$$= \frac{i}{\hbar}\frac{16L^2}{9\pi^2}\int_0^\infty \exp\left[\left(i\frac{3\hbar\pi^2}{2mL^2} - \frac{1}{\tau}\right)t'\right] dt' = \frac{i}{\hbar}\frac{16L^2}{9\pi^2}\left[\frac{2mL^2\tau}{i3\hbar\pi^2\tau - 2mL^2}\exp\left(\frac{i3\hbar\pi^2\tau - 2mL^2}{2mL^2\tau}t'\right)\right]_0^\infty$$
$$= \frac{i}{\hbar}\frac{32}{9\pi^2}\frac{mL^4\tau}{i3\hbar\pi^2\tau - 2mL^2},$$

so the transition probability is

$$|c_n^{(1)}(t)|^2 = \left(\frac{i}{\hbar}\frac{32}{9\pi^2}\frac{mL^4\tau}{i3\hbar\pi^2\tau - 2mL^2}\right)\left(\frac{i}{\hbar}\frac{32}{9\pi^2}\frac{mL^4\tau}{i3\hbar\pi^2\tau + 2mL^2}\right) = \frac{1024}{81\hbar^2}\frac{L^8\tau^2}{9\hbar^2\pi^4\tau^2 + 4m^2L^4}.$$

**Problem 2.** Consider a system of two electrons, which is described by the Hamiltonian

$$H = H_a + H_b + V, \qquad H_i = \frac{\mathbf{p}_i^2}{2m} - \frac{Z\alpha\hbar c}{r_i}, \qquad V = \frac{\alpha\hbar c}{r_{ab}}.$$

Here, we label two electrons by $i = a, b$; $r_i = |\mathbf{x}_i|$ and $r_{ab} = |\mathbf{x}_a - \mathbf{x}_b|$ where $\mathbf{x}_i$ is the spatial coordinate for electron $i$; and $Z$ and $\alpha$ are constants. To find an approximate ground state of $H$, let us try a variational wave function

$$\Psi(\mathbf{x}_a, \mathbf{x}_b) = \frac{A}{4\pi} e^{-B(r_a+r_b)},$$

where $A$ is a normalization constant and $B$ is your variational parameter.

**2.1** Compute the variational energy for the given variational parameter $B$.

**Solution.** The general expression for the variational energy $\bar{H}$ is (5.4.1) in Sakurai:

$$\bar{H} = \frac{\langle\tilde{0}|H|\tilde{0}\rangle}{\langle\tilde{0}|\tilde{0}\rangle}, \tag{2}$$

where $|\tilde{0}\rangle$ is our trial ket.

For this problem, the numerator of (2) is

$$\begin{aligned}
\langle\tilde{0}|H|\tilde{0}\rangle = \langle\Psi|H|\Psi\rangle &= \iint \langle\Psi|\mathbf{x}_a, \mathbf{x}_b\rangle \langle\mathbf{x}_a, \mathbf{x}_b|H|\mathbf{x}'_a, \mathbf{x}'_b\rangle \langle\mathbf{x}'_a, \mathbf{x}'_b|\Psi\rangle \\
&= \iint\iint \Psi(\mathbf{x}_a, \mathbf{x}_b) \langle\mathbf{x}_a, \mathbf{x}_b|H|\mathbf{x}'_a, \mathbf{x}'_b\rangle \Psi(\mathbf{x}'_a, \mathbf{x}'_b)\, d^3\mathbf{x}_a\, d^3\mathbf{x}_b\, d^3\mathbf{x}'_a\, d^3\mathbf{x}'_b\,,
\end{aligned}$$

where

$$H = \frac{\mathbf{p}_a^2}{2m} + \frac{\mathbf{p}_b^2}{2m} - \frac{Z\alpha\hbar c}{|\mathbf{x}_a|} - \frac{Z\alpha\hbar c}{|\mathbf{x}_b|} + \frac{\alpha\hbar c}{|\mathbf{x}_a - \mathbf{x}_b|},$$

so we have five integrals. For the first,

$$\begin{aligned}
&\frac{A^2}{32\pi^2 m} \iint\iint e^{-B(r_a+r_b)} \langle\mathbf{x}_a, \mathbf{x}_b|\mathbf{p}_a^2|\mathbf{x}'_a, \mathbf{x}'_b\rangle^2 e^{-B(r'_a+r'_b)}\, d^3\mathbf{x}_a\, d^3\mathbf{x}_b\, d^3\mathbf{x}'_a\, d^3\mathbf{x}'_b \\
&\quad= \frac{A^2}{32\pi^2 m} \iint\iint e^{-B(r_a+r_b)} \left(i^2\hbar^2 \delta(\mathbf{x}_a - \mathbf{x}'_a)\delta(\mathbf{x}_b - \mathbf{x}'_b)\nabla^2_{a'}\right) e^{-B(r'_a+r'_b)}\, d^3\mathbf{x}_a\, d^3\mathbf{x}_b\, d^3\mathbf{x}'_a\, d^3\mathbf{x}'_b \\
&\quad= -\frac{A^2\hbar^2}{2m} \iint e^{-B(r_a+r_b)} \left(\frac{\partial^2}{\partial r_a^2} e^{-B(r_a+r_b)}\right) r_a^2 r_b^2\, dr_a\, dr_b = -\frac{A^2 B^2\hbar^2}{2m} \int_0^\infty r_a^2 e^{-2Br_a}\, dr_a \int_0^\infty r_b^2 e^{-2Br_b}\, dr_b \\
&\quad= -\frac{A^2\hbar^2}{32B^4 m},
\end{aligned}$$

where we have used

$$\begin{aligned}
\int_0^\infty r^2 e^{-2Br}\, dr &= \left[-\frac{r^2 e^{-2Br}}{2B}\right]_0^\infty + \frac{1}{B}\int_0^\infty r e^{-2Br}\, dr = \frac{1}{B}\left[-\frac{r e^{-2Br}}{2B}\right]_0^\infty + \frac{1}{2B^2}\int_0^\infty e^{-2Br}\, dr = \frac{1}{2B^2}\left[-\frac{e^{-2Br}}{2B}\right]_0^\infty \\
&= \frac{1}{4B^3}.
\end{aligned}$$

For the second integral, we also have

$$\frac{A^2}{16\pi^2}\frac{1}{2m} \iint\iint e^{-B(r_a+r_b)} \langle\mathbf{x}_a, \mathbf{x}_b|\mathbf{p}_b^2|\mathbf{x}'_a, \mathbf{x}'_b\rangle^2 e^{-B(r'_a+r'_b)}\, d^3\mathbf{x}_a\, d^3\mathbf{x}_b\, d^3\mathbf{x}'_a\, d^3\mathbf{x}'_b = -\frac{A^2\hbar^2}{32B^4 m}.$$

For the third integral,

$$\begin{aligned}
&-\frac{Z\alpha\hbar c}{16\pi^2}\iint\iint e^{-B(r_a+r_b)}\left\langle \mathbf{x}_a,\mathbf{x}_b\right|\frac{1}{|\mathbf{x}_a|}\left|\mathbf{x}'_a,\mathbf{x}'_b\right\rangle e^{-B(r'_a+r'_b)}\,d^3\mathbf{x}_a\,d^3\mathbf{x}_b\,d^3\mathbf{x}'_a\,d^3\mathbf{x}'_b \\
&\quad=-\frac{Z\alpha\hbar c}{16\pi^2}\iint\iint e^{-B(r_a+r_b)}\left(\delta(\mathbf{x}_a-\mathbf{x}'_a)\delta(\mathbf{x}_b-\mathbf{x}'_b)\frac{1}{|\mathbf{x}_a|}\right)e^{-B(r'_a+r'_b)}\,dr_a\,dr_b\,dr'_a\,dr'_b \\
&\quad=-A^2Z\alpha\hbar c\iint\frac{e^{-2B(r_a+r_b)}}{r_a}r_a^2r_b^2\,dr_a\,dr_b=-A^2Z\alpha\hbar c\int_0^\infty r_ae^{-2Br_a}\,dr_a\int_0^\infty r_b^2e^{-2Br_b}\,dr_b \\
&\quad=-\frac{A^2Z\alpha\hbar c}{16B^5}.
\end{aligned}$$

For the fourth integral, we also have

$$-\frac{Z\alpha\hbar c}{16\pi^2}\iint\iint e^{-B(r_a+r_b)}\left\langle \mathbf{x}_a,\mathbf{x}_b\right|\frac{1}{|\mathbf{x}_b|}\left|\mathbf{x}'_a,\mathbf{x}'_b\right\rangle e^{-B(r'_a+r'_b)}\,d^3\mathbf{x}_a\,d^3\mathbf{x}_b\,d^3\mathbf{x}'_a\,d^3\mathbf{x}'_b=-\frac{A^2Z\alpha\hbar c}{16B^5}.$$

For the fifth integral, we will orient our coordinate system such that $\mathbf{x}_b$ points in the $z$ direction and stipulate that $r_a > r_b$. Then

$$\frac{1}{|\mathbf{x}_a-\mathbf{x}_b|}=\frac{1}{\sqrt{\mathbf{x}_a^2-2\mathbf{x}_a\cdot\mathbf{x}_b+\mathbf{x}_b^2}}=\frac{1}{\sqrt{r_a^2-2r_ar_b\cos\theta_a+r_b^2}},$$

and so

$$\begin{aligned}
&\frac{\alpha\hbar c}{16\pi^2}\iint\iint e^{-B(r_a+r_b)}\left\langle \mathbf{x}_a,\mathbf{x}_b\right|\frac{1}{|\mathbf{x}_a-\mathbf{x}_b|}\left|\mathbf{x}'_a,\mathbf{x}'_b\right\rangle e^{-B(r'_a+r'_b)}\,d^3\mathbf{x}_a\,d^3\mathbf{x}_b\,d^3\mathbf{x}'_a\,d^3\mathbf{x}'_b \\
&\quad=\frac{A^2\alpha\hbar c}{16\pi^2}\iint\iint e^{-B(r_a+r_b)}\left(\delta(\mathbf{x}_a-\mathbf{x}'_a)\delta(\mathbf{x}_b-\mathbf{x}'_b)\frac{1}{|\mathbf{x}_a-\mathbf{x}_b|}\right)e^{-B(r'_a+r'_b)}\,d^3\mathbf{x}_a\,d^3\mathbf{x}_b\,d^3\mathbf{x}'_a\,d^3\mathbf{x}'_b \\
&\quad=\frac{A^2\alpha\hbar c}{2}\int_0^\infty\int_{-1}^1\int_0^\infty\frac{e^{-2B(r_a+r_b)}}{\sqrt{r_a^2-2r_ar_b\cos\theta_a+r_b^2}}r_a^2r_b^2\,dr_a\,d(\cos\theta_a)\,dr_b \\
&\quad=\frac{A^2\alpha\hbar c}{2}\int_0^\infty\int_0^\infty r_a^2r_b^2e^{-2B(r_a+r_b)}\int_{-1}^1\frac{d(\cos\theta_a)}{\sqrt{r_a^2-2r_ar_b\cos\theta_a+r_b^2}}\,dr_a\,dr_b\,. \qquad (3)
\end{aligned}$$

For the innermost integral, let $u=r_a^2-2r_ar_b\cos\theta_a+r_b^2$. Then

$$d(\cos\theta_a)=-\frac{du}{2r_ar_b},$$

and we are integrating from $r_a^2+2r_ar_b+r_b^2=(r_a+r_b)^2$ to $r_a^2-2r_ar_b+r_b^2=(r_a-r_b)^2$. So the innermost integral becomes

$$\begin{aligned}
\int_{-1}^1\frac{d(\cos\theta_a)}{\sqrt{r_a^2-2r_ar_b\cos\theta_a+r_b^2}}&=\frac{1}{2r_ar_b}\int_{(r_a-r_b)^2}^{(r_a+r_b)^2}\frac{du}{\sqrt{u}}=\frac{1}{2r_ar_b}\Big[2\sqrt{u}\Big]_{(r_a-r_b)^2}^{(r_a+r_b)^2}=\frac{|r_a+r_b|-|r_a-r_b|}{r_ar_b} \\
&=\frac{r_a+r_b-r_a+r_b}{r_ar_b}=\frac{2}{r_a},
\end{aligned}$$

where we have used $r_a, r_b > 0$ and our assumption that $r_a > r_b$. Picking up from (3), we now have

$$\begin{aligned}
&\frac{A^2\alpha\hbar c}{16\pi^2}\iint\iint e^{-B(r_a+r_b)}\left\langle \mathbf{x}_a,\mathbf{x}_b\right|\frac{1}{|\mathbf{x}_a-\mathbf{x}_b|}\left|\mathbf{x}'_a,\mathbf{x}'_b\right\rangle e^{-B(r'_a+r'_b)}\,d^3\mathbf{x}_a\,d^3\mathbf{x}_b\,d^3\mathbf{x}'_a\,d^3\mathbf{x}'_b \\
&\quad=A^2\alpha\hbar c\int_0^\infty r_ae^{-2Br_a}\,dr_a\int_0^\infty r_b^2e^{-2Br_b}\,dr_b=\frac{A^2\alpha\hbar c}{16B^5}.
\end{aligned}$$

Putting this all together,

$$\langle\tilde{0}|H|\tilde{0}\rangle = \frac{A^2\alpha\hbar c}{16B^5} - \frac{A^2B\hbar^2/m}{16B^5} - \frac{2A^2Z\alpha\hbar c}{16B^5} = \frac{1}{16B^5}\left((1-2Z)A^2\alpha\hbar c - \frac{A^2B\hbar^2}{m}\right).$$

For the denominator of (2),

$$\begin{aligned}\langle\tilde{0}|\tilde{0}\rangle &= \frac{1}{16\pi^2}\iint \langle\Psi|\mathbf{x}_a,\mathbf{x}_b\rangle\langle\mathbf{x}_a,\mathbf{x}_b|\Psi\rangle\, d^3\mathbf{x}_a\, d^3\mathbf{x}_b = \iint e^{-B(r_a+r_b)}e^{-B(r_a+r_b)}r_a^2r_b^2\, dr_a\, dr_b \\ &= \int_0^\infty r_a^2e^{-2Br_a}\, dr_a \int_0^\infty r_b^2 e^{-2Br_b}\, dr_b = \frac{1}{16B^6}.\end{aligned}$$

Finally,

$$\bar{H} = A^2B(1-2Z)\alpha\hbar c - \frac{A^2B^2\hbar^2}{m}. \tag{4}$$

**2.2** By minimizing the variational energy, find the optimal value of $B$.

**Solution.** By (5.4.9) in Sakurai, we can minimize $\bar{H}$ by setting to zero its derivative with respect to $B$. From (4), we have

$$\frac{\partial\bar{H}}{\partial B} = A^2(1-2Z)\alpha\hbar c - 2\frac{A^2B\hbar^2}{m} = 0$$

which implies

$$(1-2Z)\alpha c = 2\frac{B\hbar}{m} \implies B = \frac{1-2Z}{2\hbar}\alpha cm.$$

Substituting this back into (4),

$$\bar{H} = A^2\frac{1-2Z}{2\hbar}\alpha cm(1-2Z)\alpha\hbar c - \frac{A^2\hbar^2}{m}\left(\frac{1-2Z}{2\hbar}\alpha cm\right)^2 = \frac{A^2\alpha^2c^2m}{4}(1-2Z)^2.$$

**Problem 3.** Consider a two-dimensional harmonic oscillator described by the Hamiltonian

$$H_0 = \frac{p_x^2 + p_y^2}{2m} + m\omega^2 \frac{x^2 + y^2}{2}.$$

**3.1** How many single-particle states are there for the first excited level?

**Solution.** The Hamiltonian is separable; that is, we may write $H_0 = H_x + H_y$ where

$$H_x = \frac{p_x^2}{2m} + m\omega^2 \frac{x^2}{2}, \qquad H_y = \frac{p_y^2}{2m} + m\omega^2 \frac{y^2}{2},$$

which are both one-dimensional oscillators. Thus, the energy of each is given by (A.4.4) in Sakurai:

$$E = \hbar\omega \left(n + \frac{1}{2}\right), \qquad n = 0, 1, 2, \ldots$$

So the total energy for $H_0$ is

$$E_0 = E_x + E_y = \hbar\omega(n_x + n_y + 1), \qquad n_x, n_y = 0, 1, 2, \ldots$$

Ignoring spin, for the first excited level we may have

$$|n_x, n_y\rangle = \begin{cases} |0, 1\rangle, \\ |1, 0\rangle. \end{cases}$$

This gives us *two* single-particle states.

If we assume that the single particle is an electron, we have an additional spin degree of freedom, which we denote by $s$. Then the possible configurations are

$$|n_x, n_y, s\rangle = \begin{cases} |0, 1, +\rangle, \\ |0, 1, -\rangle, \\ |1, 0, +\rangle, \\ |1, 0, -\rangle, \end{cases}$$

which gives us *four* single-particle states.

**3.2** Write down the many-body ground state for two electrons (with spin). What is the eigenvalue of $\mathbf{S}^2 = (\mathbf{S}_1 + \mathbf{S}_2)^2$ for this state? Here $\mathbf{S}_i$ are the spin operators of the electrons.

**Solution.** For two electrons, the Hamiltonian is

$$H_0 = \frac{{p_x}_1^2 + {p_y}_1^2}{2m} + \frac{{p_x}_2^2 + {p_y}_2^2}{2m} + m\omega^2 \frac{x_1^2 + y_1^2}{2} + m\omega^2 \frac{x_2^2 + y_2^2}{2}.$$

From (6.3.2) in Sakurai, the Hamiltonian commutes with $\mathbf{S}^2$—that is, $[\mathbf{S}^2, H_0] = 0$—so the eigenfunctions $\psi$ of $H_0$ are also eigenfunctions of $\mathbf{S}^2$. This also means the eigenfunctions are separable, and so they can be written as in (6.6.3):

$$\psi = \phi(\mathbf{x}_1, \mathbf{x}_2)\chi, \tag{5}$$

where $\mathbf{x}_i = (x_i, y_i)$ for this problem. Here, $\phi$ is given by (6.3.14),

$$\phi(\mathbf{x}_1, \mathbf{x}_2) = \frac{\omega_A(\mathbf{x}_1)\,\omega_B(\mathbf{x}_2) \pm \omega_A(\mathbf{x}_2)\,\omega_B(\mathbf{x}_1)}{\sqrt{2}} \begin{cases} \text{symmetrical,} \\ \text{antisymmetrical,} \end{cases} \tag{6}$$

where $\omega_A$ and $\omega_B$ each represent states. Next, $\chi$ is given by (6.3.4),

$$\chi(m_{s1}, m_{s2}) = \begin{cases} \chi_{++} & \text{triplet (symmetrical),} \\ \dfrac{\chi_{+-} + \chi_{-+}}{\sqrt{2}} & \text{triplet (symmetrical),} \\ \chi_{--} & \text{triplet (symmetrical),} \\ \dfrac{\chi_{+-} - \chi_{-+}}{\sqrt{2}} & \text{singlet (antisymmetrical).} \end{cases}$$

Since the two-dimensional harmonic oscillator is separable in $x$ and $y$, we can write

$$\omega(\mathbf{x}) = f_{n_x}(x)\, g_{n_y}(y),$$

where $f_{n_x}$ and $g_{n_y}$ are both eigenfunctions corresponding to levels $n$ and $n'$ of the one-dimensional harmonic oscillator Hamiltonian, given by Sakurai (A.4.3):

$$\psi_E = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2} H_n(\xi),$$

where $\xi = \sqrt{m\omega/\hbar}x$ from (A.4.2), and $H_n$ are the Hermite polynomials. Using this notation, (6) becomes

$$\phi(\mathbf{x}_1, \mathbf{x}_2) = \frac{f_{A_x}(x_1)\, g_{A_y}(y_1)\, f_{B_x}(x_2)\, g_{B_y}(y_2) \pm f_{A_x}(x_2)\, g_{A_y}(y_2)\, f_{B_x}(x_1)\, g_{B_y}(y_1)}{\sqrt{2}} \begin{cases} \text{symmetrical,} \\ \text{antisymmetrical,} \end{cases}$$

or, in Dirac notation,

$$|\phi\rangle = \frac{|A_x B_x\rangle\, |A_y B_y\rangle \pm |B_x A_x\rangle\, |B_y A_y\rangle}{\sqrt{2}} \begin{cases} \text{symmetrical,} \\ \text{antisymmetrical,} \end{cases} \tag{7}$$

where the first ket represents $|n_{x1}, n_{x2}\rangle$ and the second $|n_{y_1}, n_{y_2}\rangle$.

For the ground state, $(A_x, A_y) = (B_x, B_y) = (0, 0)$. Then (7) becomes

$$|\phi\rangle = \frac{2}{\sqrt{2}} \begin{cases} |00\rangle\, |00\rangle + |00\rangle\, |00\rangle = 2\, |00\rangle\, |00\rangle & \text{symmetrical,} \\ |00\rangle\, |00\rangle - |00\rangle\, |00\rangle = 0 & \text{antisymmetrical.} \end{cases}$$

Only the symmetrical spatial function is nonzero. For two fermions, we need the overall wavefunction to be antisymmetric, so this means we must have the spin singlet state. The ground state is then

$$|\psi\rangle = |n_{x1}, n_{x2}\rangle\, |n_{x1}, n_{y_1}\rangle\, |s_1, s_2\rangle = \frac{|00\rangle\, |00\rangle\, |{+-}\rangle - |00\rangle\, |00\rangle\, |{-+}\rangle}{\sqrt{2}},$$

where we have normalized.

The eigenvalues of $\mathbf{S}^2$ and $S^z$ are given by Sakurai (3.7.12),

$$\mathbf{S}^2 = (\mathbf{S}_1 + \mathbf{S}_2)^2 : s(s+1)\hbar, \qquad S^z = S_1^z + S_2^z : m\hbar, \tag{8}$$

where the $s$ and $m$ quantum numbers for each spinor $\chi$ are given by (3.7.15):

$$\begin{aligned} |s=1,m=1\rangle &= |{+}{+}\rangle\,, & |s=1,m=0\rangle &= \frac{|{+}{-}\rangle + |{-}{+}\rangle}{\sqrt{2}}, \\ |s=1,m=-1\rangle &= |{-}{-}\rangle\,, & |s=0,m=0\rangle &= \frac{|{+}{-}\rangle - |{-}{+}\rangle}{\sqrt{2}}. \end{aligned} \tag{9}$$

So for the singlet, as we have in the ground state, the eigenvalue of $\mathbf{S}$ is 0.

**3.3** Write down all the first excited many-body states of two electrons (with spin). Choose them to be eigenstates of the total spin operator, and compute their eigenvalues of $(\mathbf{S}_1 + \mathbf{S}_2)^2$ and $S^z = S_1^z + S_2^z$ (where $S_i^z$ is the $z$ component of the spin operator $\mathbf{S}_i$).

**Solution.** For the spatial part $\phi$ of (5), we may have

$$(A_x, A_y) = (1,0) \text{ and } (B_y, B_y) = (0,0), \qquad (A_x, A_y) = (0,1) \text{ and } (B_x, B_y) = (0,0).$$

In both cases, both the symmetric and antisymmetric cases of (7) are nontrivial:

$$\phi(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{\sqrt{2}} \begin{cases} |01\rangle\,|00\rangle \pm |10\rangle\,|00\rangle & \begin{cases}\text{symmetrical,} \\ \text{antisymmetrical,}\end{cases} \\ |00\rangle\,|01\rangle \pm |00\rangle\,|10\rangle & \begin{cases}\text{symmetrical,} \\ \text{antisymmetrical.}\end{cases} \end{cases}$$

so we will make use of both the singlet and triplet spinors. The possible states with the $\mathbf{S}$ and $S^z$ eigenvales are

$$\psi = \begin{cases} \frac{|01\rangle\,|00\rangle + |10\rangle\,|00\rangle}{\sqrt{2}} \frac{|{+}{-}\rangle - |{-}{+}\rangle}{\sqrt{2}} & \mathbf{S}:0 \quad S^z:0, \\ \frac{|01\rangle\,|00\rangle - |10\rangle\,|00\rangle}{\sqrt{2}} |{+}{+}\rangle & \mathbf{S}:1 \quad S^z:1, \\ \frac{|01\rangle\,|00\rangle - |10\rangle\,|00\rangle}{\sqrt{2}} \frac{|{+}{-}\rangle + |{-}{+}\rangle}{\sqrt{2}} & \mathbf{S}:1 \quad S^z:1, \\ \frac{|01\rangle\,|00\rangle - |10\rangle\,|00\rangle}{\sqrt{2}} |{-}{-}\rangle & \mathbf{S}:1 \quad S^z:-1, \\ \frac{|00\rangle\,|01\rangle + |00\rangle\,|10\rangle}{\sqrt{2}} \frac{|{+}{-}\rangle - |{-}{+}\rangle}{\sqrt{2}} & \mathbf{S}:0 \quad S^z:0, \\ \frac{|00\rangle\,|01\rangle - |00\rangle\,|10\rangle}{\sqrt{2}} |{+}{+}\rangle & \mathbf{S}:1 \quad S^z:1, \\ \frac{|00\rangle\,|01\rangle - |00\rangle\,|10\rangle}{\sqrt{2}} \frac{|{+}{-}\rangle + |{-}{+}\rangle}{\sqrt{2}} & \mathbf{S}:1 \quad S^z:0, \\ \frac{|00\rangle\,|01\rangle - |00\rangle\,|10\rangle}{\sqrt{2}} |{-}{-}\rangle & \mathbf{S}:1 \quad S^z:-1. \end{cases}$$

I consulted Sakurai's *Modern Quantum Mechanics*, Shankar's *Principles of Quantum Mechanics*, and Wolfram MathWorld while writing up these solutions.