1. Consider a particle of mass m attached to a rigid massless rod of fixed length R whose other end is fixed at the origin. The rod is free to rotate about the origin. Classical mechanics teaches us that the Hamiltonian of this system is given by

$$H = \frac{\vec{\boldsymbol{L}}^2}{2I}\,,$$

where $I = mR^2$ is the moment of inertia, and $\vec{\boldsymbol{L}} = \vec{\boldsymbol{r}} \times \vec{\boldsymbol{p}}$ is the angular momentum. In quantum mechanics, $\vec{\boldsymbol{L}}$ is an operator, and the Schrodinger equation for the energy levels of the rigid rotator is given by $H\,|\psi\rangle = E\,|\psi\rangle$.

(a) What are the possible energy eigenvalues of the system?

Since the eigenvalues of $\vec{\boldsymbol{L}}^2$ are $\hbar^2\ell(\ell+1)$, where $\ell = 0, 1, 2, \ldots$, it follows that the eigenvalues of $H = \vec{\boldsymbol{L}}^2/(2I)$ are $\hbar^2\ell(\ell+1)/(2I)$, where $\ell = 0, 1, 2, \ldots$.

(b) Suppose that the particle of mass m has no internal spin degree of freedom, but carries an electric charge $+e$. It is placed in a uniform magnetic field $\vec{\boldsymbol{B}}$. Using the principle of minimal substitution, write down the Schrodinger equation for the charged rigid rotator.

According to the principle of minimal substitution, we replace $\vec{\boldsymbol{p}} \longrightarrow \vec{\boldsymbol{p}} - e\vec{\boldsymbol{A}}$ in the Hamiltonian. Thus,

$$H = \frac{\left[\vec{\boldsymbol{r}} \times (\vec{\boldsymbol{p}} - e\vec{\boldsymbol{A}})\right]^2}{2I}\,. \tag{1}$$

For a uniform magnetic field, a convenient choice for $\vec{\boldsymbol{A}}$ is given by:

$$\vec{\boldsymbol{A}} = -\tfrac{1}{2}\vec{\boldsymbol{r}} \times \vec{\boldsymbol{B}}\,, \tag{2}$$

which is consistent with the Coulomb gauge condition, $\vec{\boldsymbol{\nabla}}\cdot\vec{\boldsymbol{A}} = 0$. In the coordinate representation, the momentum operator i given by $\vec{\boldsymbol{p}} = -i\hbar\vec{\boldsymbol{\nabla}}$. Hence, for any wave function ψ,

$$\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{A}}\,\psi = -i\hbar\vec{\boldsymbol{\nabla}}\cdot(\vec{\boldsymbol{A}}\psi) = -ih\left[\vec{\boldsymbol{A}}\cdot\vec{\boldsymbol{\nabla}}\psi + \psi\vec{\boldsymbol{\nabla}}\cdot\vec{\boldsymbol{A}}\right] = -i\hbar\vec{\boldsymbol{A}}\cdot\vec{\boldsymbol{\nabla}}\psi = \vec{\boldsymbol{A}}\cdot\vec{\boldsymbol{p}}\,\psi\,.$$

That is, in the Coulomb gauge, $\vec{\boldsymbol{A}}\cdot\vec{\boldsymbol{p}} = \vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{A}}$, and we do not have to worry about the relative ordering of these two operators.

We now proceed to simplify the Hamiltonian given in eq. (1). Consider two operators, $\vec{\boldsymbol{C}}$ and $\vec{\boldsymbol{D}}$ that do not commute. Using,

$$(\vec{\boldsymbol{C}} \times \vec{\boldsymbol{D}})_i = \sum_{j,k} \epsilon_{ijk} C_j D_k\,,$$

it follows that:

$$(\vec{\boldsymbol{C}}\times\vec{\boldsymbol{D}})^2=\sum_{j,k,\ell,m}\epsilon_{ijk}\epsilon_{i\ell m}C_jD_kC_\ell D_m=\sum_{j,k,\ell,m}(\delta_{jl}\delta_{km}-\delta_{jm}\delta_{k\ell})C_jD_kC_\ell D_m$$

$$=\sum_{j,k}(C_jD_kC_jD_k-C_jD_kC_kD_j)$$

$$=\sum_{j,k}C_jD_kC_jD_k-\sum_j C_j(\vec{\boldsymbol{D}}\cdot\vec{\boldsymbol{C}})D_j\,,$$

where I have been careful to keep track of the order of the operators. Applying this result with $\vec{\boldsymbol{C}}\equiv\vec{\boldsymbol{r}}$ and $\vec{\boldsymbol{D}}\equiv\vec{\boldsymbol{p}}-e\vec{\boldsymbol{A}}$, one obtains:

$$\left[\vec{\boldsymbol{r}}\times(\vec{\boldsymbol{p}}-e\vec{\boldsymbol{A}})\right]^2=\sum_{j,k}r_j(p-eA)_k\,r_j(p-eA)_k-\sum_j r_j\left[(\vec{\boldsymbol{p}}-e\vec{\boldsymbol{A}})\cdot\vec{\boldsymbol{r}}\right](p-eA)_j\,.$$

If we now make use of the expression for $\vec{\boldsymbol{A}}$ given in eq. (2), the second term above can be simplified, since

$$\vec{\boldsymbol{A}}\cdot\vec{\boldsymbol{r}}=-\tfrac{1}{2}(\vec{\boldsymbol{r}}\times\vec{\boldsymbol{B}})\cdot\vec{\boldsymbol{r}}=0\,,$$

since $\vec{\boldsymbol{r}}$ is perpendicular to $\vec{\boldsymbol{r}}\times\vec{\boldsymbol{B}}$. Hence, $(\vec{\boldsymbol{p}}-e\vec{\boldsymbol{A}})\cdot\vec{\boldsymbol{r}}=\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{r}}$. Hence,

$$\left[\vec{\boldsymbol{r}}\times(\vec{\boldsymbol{p}}-e\vec{\boldsymbol{A}})\right]^2=(\vec{\boldsymbol{r}}\times\vec{\boldsymbol{p}})^2-e\sum_{j,k}r_j(A_kr_jp_k+p_kr_jA_k)+e\sum_j r_j(\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{r}})A_j+e^2\sum_{j,k}r_jA_kr_jA_k\,. \tag{3}$$

Since $\vec{\boldsymbol{A}}$ is a function of $\vec{\boldsymbol{r}}$ (and not of $\vec{\boldsymbol{p}}$), it follows that $\vec{\boldsymbol{A}}$ commutes with $\vec{\boldsymbol{r}}$. However, $\vec{\boldsymbol{p}}$ does not commute with $\vec{\boldsymbol{r}}$. Instead,

$$[r_j\,,\,p_k]=i\hbar\delta_{jk}\,,$$

or equivalently,

$$r_jp_k=p_kr_j+i\hbar\delta_{jk}\,.$$

As a result,

$$\sum_j r_j(\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{r}})A_j=\sum_{j,k}r_jp_kr_kA_j=\sum_{j,k}(p_kr_j+i\hbar\delta_{jk})r_kA_j=(\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{r}}+i\hbar)\vec{\boldsymbol{r}}\cdot\vec{\boldsymbol{A}}=0\,, \tag{4}$$

since $[r_j\,,\,r_k]=0$ and $\vec{\boldsymbol{r}}\cdot\vec{\boldsymbol{A}}=\vec{\boldsymbol{A}}\cdot\vec{\boldsymbol{r}}=0$ as previously noted for a uniform magnetic field in the Coulomb gauge. Next, we examine:

$$\sum_{j,k}r_jp_kr_jA_k=\sum_{j,k}r_j(r_jp_k-i\hbar\delta_{jk})A_k=r^2\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{A}}-i\hbar\vec{\boldsymbol{r}}\cdot\vec{\boldsymbol{A}}=r^2\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{A}}\,, \tag{5}$$

where we have again used $\vec{\boldsymbol{r}}\cdot\vec{\boldsymbol{A}}=0$. As usual, we denote $r^2\equiv\vec{\boldsymbol{r}}\cdot\vec{\boldsymbol{r}}$. Finally, noting that $[A_k\,,\,r_j]=0$, it follows that:

$$\sum_{j,k}r_jA_kr_jp_k=r^2\vec{\boldsymbol{A}}\cdot\vec{\boldsymbol{p}}\,. \tag{6}$$

Inserting the results of eqs. (4)–(6) into eq. (3), one obtains:

$$\begin{aligned}\left[\vec{\boldsymbol{r}}\times(\vec{\boldsymbol{p}}-e\vec{\boldsymbol{A}})\right]^2 &= (\vec{\boldsymbol{r}}\times\vec{\boldsymbol{p}})^2 - er^2\left(\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{A}}+\vec{\boldsymbol{A}}\cdot\vec{\boldsymbol{p}}\right)+e^2r^2\vec{\boldsymbol{A}}^2\\ &= \vec{\boldsymbol{L}}^2 - 2er^2\vec{\boldsymbol{A}}\cdot\vec{\boldsymbol{p}}+e^2r^2\vec{\boldsymbol{A}}^2\,,\end{aligned}\tag{7}$$

where in the last step, we have used the fact that $\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{A}}=\vec{\boldsymbol{A}}\cdot\vec{\boldsymbol{p}}$ in the Coulomb gauge. We now substitute $\vec{\boldsymbol{A}}=\frac{1}{2}\vec{\boldsymbol{r}}\times\vec{\boldsymbol{B}}$ (appropriate for a uniform magnetic field), and note that:

$$\begin{aligned}\vec{\boldsymbol{A}}\cdot\vec{\boldsymbol{p}} &= -\tfrac{1}{2}(\vec{\boldsymbol{r}}\times\vec{\boldsymbol{B}})\cdot\vec{\boldsymbol{p}}=\tfrac{1}{2}(\vec{\boldsymbol{B}}\times\vec{\boldsymbol{r}})\cdot\vec{\boldsymbol{p}}=\tfrac{1}{2}\vec{\boldsymbol{B}}\cdot(\vec{\boldsymbol{r}}\times\vec{\boldsymbol{p}})=\tfrac{1}{2}\vec{\boldsymbol{B}}\cdot\vec{\boldsymbol{L}}\\ \vec{\boldsymbol{A}}^2 &= \tfrac{1}{4}(\vec{\boldsymbol{r}}\times\vec{\boldsymbol{B}})^2=\tfrac{1}{4}\left[r^2\vec{\boldsymbol{B}}^2-(\vec{\boldsymbol{r}}\cdot\vec{\boldsymbol{B}})^2\right].\end{aligned}$$

Inserting these results into eq. (7), we end up with

$$\boxed{H=\frac{1}{2I}\left\{\vec{\boldsymbol{L}}^2-er^2\vec{\boldsymbol{B}}\cdot\vec{\boldsymbol{L}}+\tfrac{1}{4}e^2r^2\left[r^2\vec{\boldsymbol{B}}^2-(\vec{\boldsymbol{r}}\cdot\vec{\boldsymbol{B}})^2\right]\right\}.}$$

The time-independent Schrodinger equation then reads:

$$\frac{1}{2I}\left\{\vec{\boldsymbol{L}}^2-er^2\vec{\boldsymbol{B}}\cdot\vec{\boldsymbol{L}}+\tfrac{1}{4}e^2r^2\left[r^2\vec{\boldsymbol{B}}^2-(\vec{\boldsymbol{r}}\cdot\vec{\boldsymbol{B}})^2\right]\right\}\psi=E\psi\,,$$

where H is given above and $\vec{\boldsymbol{L}}\psi\equiv-i\hbar\vec{\boldsymbol{r}}\times\vec{\boldsymbol{\nabla}}\psi$.

(c) Compute the energy levels of the system described in part (b), assuming that the magnetic field is weak (i.e., assume that the term in the Hamiltonian that is quadratic in $\vec{\boldsymbol{B}}$ can be neglected).

If the magnetic field is weak, one can neglect the term in H that is quadratic in the B-field. Thus, one can use the approximate Hamiltonian,

$$H=\frac{1}{2I}\left[\vec{\boldsymbol{L}}^2-er^2\vec{\boldsymbol{B}}\cdot\vec{\boldsymbol{L}}\right].$$

One is free to choose the z-axis to lie along $\vec{\boldsymbol{B}}$, so that $\vec{\boldsymbol{B}}=B\hat{\boldsymbol{z}}$. Moreover, the length of the co-ordinate $\vec{\boldsymbol{r}}$ is fixed, $r=R$, since by assumption the rigid rotator has a fixed length. The moment of inertia of the rigid rotator is $I=mR^2$. Hence,

$$H=\frac{\vec{\boldsymbol{L}}^2}{2mR^2}-\frac{eBL_z}{2m}\,.$$

The eigenstates of H are simultaneous eigenstates of $\vec{\boldsymbol{L}}^2$ and L_z. Since the possible eigenvalues of L_z are $\hbar m_\ell$, where

$$m_\ell=-\ell\,,\,-\ell+1\,,\,\ldots\,,\,\ell-1\,,\,\ell\,,$$

it follows that the energy levels of the charged rigid rotator in a weak uniform magnetic field are given by:

$$\boxed{E = \frac{\hbar^2 \ell(\ell+1)}{2mR^2} - \frac{e\hbar B}{2m} m_\ell \qquad \begin{array}{c} \ell = 0\,,\,1\,,\,2\,,\,\ldots \\ m_\ell = -\ell\,,\,-\ell+1\,,\,\ldots\,,\,\ell-1\,,\,\ell \end{array}}$$

Of course, this is the Zeeman effect.

REMARK: The model of the rigid rotator is a good one for diatomic molecules. Thus, the above result provides a model for the behavior of the rotational levels of diatomic molecules in the presence of a weak uniform magnetic field.

2. Positronium is a bound state of two spin 1/2 particles: an electron (e^-) and a positron (e^+). Consider the Hamiltonian for the system, where we focus only on the spin degrees of freedom. In the presence of a uniform external magnetic field, we may take:

$$H = A(I - \vec{\boldsymbol{\sigma}}_{\mathbf{1}} \cdot \vec{\boldsymbol{\sigma}}_{\mathbf{2}}) + \mu_B(\vec{\boldsymbol{\sigma}}_{\mathbf{1}} - \vec{\boldsymbol{\sigma}}_{\mathbf{2}}) \cdot \vec{\boldsymbol{B}}\,,$$

where A is a constant, I is the identity matrix in the direct product space of the two spin-$\frac{1}{2}$ Hilbert spaces, $\mu_B \equiv e\hbar/(2mc)$, and m is the electron mass. The labels 1 and 2 refer to the e^- and the e^+ respectively.

(a) Consider separately the case of zero magnetic field and the case of a uniform magnetic field pointing in the z-direction. In each case, list the complete set of simultaneously commuting angular momentum operators that also commute with the Hamiltonian H given above.

Using $\vec{\boldsymbol{S}}_{\boldsymbol{i}} \equiv \frac{1}{2}\hbar \vec{\boldsymbol{\sigma}}_{\boldsymbol{i}}$ $(i = 1, 2)$, we can rewrite H as:

$$H = A\left[I - \frac{4}{\hbar^2}\vec{\boldsymbol{S}}_{\mathbf{1}} \cdot \vec{\boldsymbol{S}}_{\mathbf{2}}\right] + \frac{e}{m}\left(\vec{\boldsymbol{S}}_{\mathbf{1}} - \vec{\boldsymbol{S}}_{\mathbf{2}}\right) \cdot \vec{\boldsymbol{B}}\,.$$

The total spin operator is $\vec{\boldsymbol{S}} \equiv \vec{\boldsymbol{S}}_{\mathbf{1}} + \vec{\boldsymbol{S}}_{\mathbf{2}}$. Squaring this expression and solving for $\vec{\boldsymbol{S}}_{\mathbf{1}} \cdot \vec{\boldsymbol{S}}_{\mathbf{2}}$, one obtains:

$$\vec{\boldsymbol{S}}_{\mathbf{1}} \cdot \vec{\boldsymbol{S}}_{\mathbf{2}} = \tfrac{1}{2}\left[\vec{\boldsymbol{S}}^2 - \vec{\boldsymbol{S}}_{\mathbf{1}}^2 - \vec{\boldsymbol{S}}_{\mathbf{2}}^2\right]\,.$$

First, suppose that $\vec{\boldsymbol{B}} = 0$. Then H commutes with $\vec{\boldsymbol{S}}^2$, S_z, $\vec{\boldsymbol{S}}_{\mathbf{1}}^2$ and $\vec{\boldsymbol{S}}_{\mathbf{2}}^2$. Note that H does not commute with any of the components of $\vec{\boldsymbol{S}}_{\mathbf{1}}$ and $\vec{\boldsymbol{S}}_{\mathbf{2}}$. For example,

$$[S_{1i}\,,\,\vec{\boldsymbol{S}}_{\mathbf{1}} \cdot \vec{\boldsymbol{S}}_{\mathbf{2}}] = \sum_j [S_{1i}\,,\,S_{1j}]S_{2j} = i\hbar \sum_{j,k} \epsilon_{ijk} S_{1k} S_{2j} \neq 0\,.$$

Next, if $\vec{\boldsymbol{B}} \equiv B\hat{\boldsymbol{z}}$ (without loss of generality, we are free to choose the z-axis to lie in the direction of the B-field), then H still commutes with S_z, $\vec{\boldsymbol{S}}_{\mathbf{1}}^2$ and $\vec{\boldsymbol{S}}_{\mathbf{2}}^2$.

However, H no longer commutes with $\vec{\boldsymbol{S}}^2$. For example,

$$[\vec{\boldsymbol{S}}^2\,,\,(S_1-S_2)_i] = [\vec{\boldsymbol{S}}_{\boldsymbol{1}}^2+\vec{\boldsymbol{S}}_{\boldsymbol{2}}^2+2\,\vec{\boldsymbol{S}}_{\boldsymbol{1}}\cdot\vec{\boldsymbol{S}}_{\boldsymbol{2}}\,,\,(S_1-S_2)_i] = 2\sum_j [S_{1j}S_{2j}\,,\,(S_1-S_2)_i]$$

$$= 2S_{2j}[S_{1j}\,,\,S_{1i}] - 2S_{1j}[S_{2j}\,,\,S_{2i}]$$

$$= 2i\hbar\sum_{j,k}\epsilon_{jik}\,(S_{2j}S_{1k}-S_{1j}S_{2k}) = 4i\hbar\sum_{j,k}\epsilon_{ijk}S_{1j}S_{2k} \neq 0\,.$$

(b) In zero magnetic field, a transition is observed to occur from the $S=1$ state to the $S=0$ state (which is the ground state). The emitted photon is observed to have a frequency of 2×10^5 MHz. Compute the energy levels of the system (for $B=0$), and then evaluate the constant A that appears in the Hamiltonian.

If $\vec{\boldsymbol{B}}=0$, then the eigenstates of H can be chosen to be simultaneous eigenstates of $\vec{\boldsymbol{S}}^2$, S_z, $\vec{\boldsymbol{S}}_{\boldsymbol{1}}^2$ and $\vec{\boldsymbol{S}}_{\boldsymbol{2}}^2$. These eigenstates are denoted by $|s\,,\,m_s\rangle$, where the possible values of s and m_s are: $s=1$ and $m_s=+1\,,\,0\,,\,-1$ corresponding to the triplet spin state, and $s=0$ and $m_s=0$ corresponding to the singlet spin state. In the case of zero orbital angular momentum ($\ell=0$), the triplet state is denoted by ${}^3S_1$ and the singlet state by ${}^1S_0$. The latter is the ground state of the system.

Using the results of part (a), the Hamiltonian in the case of zero external magnetic field can be written as:

$$H = A\left[I - \frac{2}{\hbar^2}\left(\vec{\boldsymbol{S}}^2 - \vec{\boldsymbol{S}}_{\boldsymbol{1}}^2 - \vec{\boldsymbol{S}}_{\boldsymbol{2}}^2\right)\right]\,.$$

Using

$$\vec{\boldsymbol{S}}^2\,|s\,,\,m_s\rangle = \hbar^2 s(s+1)\,|s\,,\,m_s\rangle\ ,$$

$$\vec{\boldsymbol{S}}_{\boldsymbol{1}}{}^2\,|s\,,\,m_s\rangle = \tfrac{3}{4}\hbar^2\,|s\,,\,m_s\rangle\ ,$$

$$\vec{\boldsymbol{S}}_{\boldsymbol{2}}{}^2\,|s\,,\,m_s\rangle = \tfrac{3}{4}\hbar^2\,|s\,,\,m_s\rangle\ ,$$

where the latter two results above are a consequence of the fact the the electron and positron are both spin-$\frac{1}{2}$ particles, it follows that

$$H\,|s\,,\,m_s\rangle = A\big\{1-2\left[s(s+1)-\tfrac{3}{2}\right]\big\}\,|s\,,\,m_s\rangle = \begin{cases} 0 & , \quad \text{for} \ \ s=1\,, \\ 4A\,|s\,,\,m_s\rangle & , \quad \text{for} \ \ s=0\,. \end{cases}$$

That is, the energies of the ${}^3S_1$ and ${}^1S_0$ states are given by

$$E = \begin{cases} 0 & , \quad \text{for the} \ \ {}^3S_1 \ \ \text{state}\,, \\ 4A & , \quad \text{for the} \ \ {}^1S_0 \ \ \text{state}\,. \end{cases} \tag{8}$$

A photon with the a frequency of $\nu \equiv 2 \times 10^5$ MHz is observed in a transition from the ${}^3S_1$ state to the ${}^1S_0$ ground state. Since,

$$\Delta E \equiv E({}^3S_1) - E({}^1S_0) = h\nu = -4A\,,$$

it follows that

$$A = -\tfrac{1}{4}h\nu = -\tfrac{1}{4}(4.136 \times 10^{-15}\ \text{eV–sec})(2 \times 10^{11}\ \text{sec}^{-1}) = -2.068 \times 10^{-4}\ \text{eV}\,.$$

3. Liboff, problem 12.5 on page 584.

Liboff defines the term *multiplicity* to be the number of possible j values for a given ℓ and s. As shown on pp. 581–583 of Liboff, the multiplicity is equal to $2s+1$ if $s \le \ell$ and $2\ell+1$ for $s \ge \ell$ (the definitions agree in the case of $\ell = s$).

(a) ${}^3D_2$ means $\ell = 2$, $s = 1$ and $j = 2$. The multiplicity is $2s + 1 = 3$.

(b) ${}^4P_{5/2}$ means $\ell = 1$, $s = 3/2$ and $j = 5/2$. The multiplicity is $2\ell + 1 = 3$.

(c) ${}^2F_{7/2}$ means $\ell = 3$, $s = 1/2$ and $j = 7/2$. The multiplicity is $2s + 1 = 2$.

(d) ${}^3G_3$ means $\ell = 4$, $s = 1$ and $j = 3$. The multiplicity is $2s + 1 = 3$.

4. Liboff, problem 13.4 on page 689.

(a) The unperturbed Hamiltonian is

$$H^{(0)}(x) = \begin{cases} 0\,, & \text{for } \ |x| \le L/2\,, \\ \infty\,, & \text{for } \ |x| \ge L/2\,, \end{cases}$$

and the perturbation is

$$H^{(1)}(x) = \begin{cases} V_0\,, & \text{for } \ |x| \le a/2\,, \\ 0\,, & \text{for } \ |x| \le a/2\,, \end{cases}$$

where $0 < a < L$. First, we need to solve for the energy eigenvalues and the corresponding eigenfunctions of $H^{(0)}$. These are given in eq. (6.100) on p. 179 of Liboff:

$$E_n^{(0)} = \frac{\hbar^2\pi^2 n^2}{2mL^2}\,,$$

and

$$\left|n^{(0)}\right\rangle = \begin{cases} \sqrt{\dfrac{2}{L}}\sin\left(\dfrac{n\pi x}{L}\right)\,, & \text{for } \ n = 2\,,\,4\,,\,6\,,\,\ldots\,, \\ \sqrt{\dfrac{2}{L}}\cos\left(\dfrac{n\pi x}{L}\right)\,, & \text{for } \ n = 1\,,\,3\,,\,5\,,\,\ldots\,. \end{cases} \tag{9}$$

The first order energy shift for the $n = 2$ energy level is given by

$$E_2^{(1)} = \big\langle 2^{(0)}\big|\, H^{(1)}\, \big|2^{(0)}\big\rangle = \frac{2V_0}{L}\int_{-a/2}^{a/2} \sin^2\left(\frac{2\pi x}{L}\right)\, dx = \frac{V_0 a}{L}\left[1 - \frac{\sin(2\pi a/L)}{(2\pi a/L)}\right].$$

That is, the corrected second eigenenergy to first order in the perturbation is given by:

$$E_2 = \frac{2\hbar^2\pi^2}{mL^2} + \frac{V_0 a}{L}\left[1 - \frac{\sin(2\pi a/L)}{(2\pi a/L)}\right].$$

The corrected eigenfunction to first order in the perturbation, $\big|2^{(0)}\big\rangle + \big|2^{(1)}\big\rangle$, is obtained using

$$\big|2^{(1)}\big\rangle = \sum_{n\neq 2} \frac{\big|n^{(0)}\big\rangle\,\big\langle n^{(0)}\big|\, H^{(1)}\, \big|2^{(0)}\big\rangle}{E_2^{(0)} - E_n^{(0)}}\,.$$

Thus, we compute

$$\big\langle n^{(0)}\big|\, H^{(1)}\, \big|2^{(0)}\big\rangle = \begin{cases} \dfrac{2V_0}{L}\displaystyle\int_{-a/2}^{a/2} \sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)\,, & \text{for } n \text{ even}\,, \\[2ex] \dfrac{2V_0}{L}\displaystyle\int_{-a/2}^{a/2} \sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{n\pi x}{L}\right)\,, & \text{for } n \text{ odd}\,, \end{cases}$$

where the case of $n = 2$ is excluded. The above integrals are easily evaluated:

$$\frac{2V_0}{L}\int_{-a/2}^{a/2} \sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right) = \frac{2V_0}{\pi}\left[\frac{\sin\left(\dfrac{(n-2)\pi a}{2L}\right)}{n-2} - \frac{\sin\left(\dfrac{(n+2)\pi a}{2L}\right)}{n+2}\right],$$

$$\int_{-a/2}^{a/2} \sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{n\pi x}{L}\right) = 0\,.$$

In evaluating the first integral above, we set $u = \pi x/L$ and employed the trigonometric identity:

$$\sin(2u)\sin(nu) = \tfrac{1}{2}\Big[\cos[(n-2)u] - \cos[(n+2)u]\Big].$$

The second integral above vanishes, since the integrand is an odd function with respect to $x \longrightarrow -x$. Hence,

$$\big|2^{(1)}\big\rangle = \frac{2V_0}{\pi E_1^{(0)}}\sqrt{\frac{2}{L}}\sum_{n=4,6,\ldots}\left[\frac{\sin\left(\dfrac{(n-2)\pi a}{2L}\right)}{n-2} - \frac{\sin\left(\dfrac{(n+2)\pi a}{2L}\right)}{n+2}\right]\frac{\sin\left(\dfrac{n\pi x}{L}\right)}{4-n^2}\,,$$

where $E_1^{(0)} \equiv \hbar^2\pi^2/(2mL^2)$, and the sum is taken over all positive even numbers excluding $n = 2$. There is no simple closed-form expression for the sum above.

(b) In order for the approximation to be valid, the energy shift should be parametrically smaller than the unperturbed energy. Since the ratio a/L need not be particularly small, we simply require that

$$V_0 \ll \frac{\hbar^2 \pi^2}{mL^2} \,,$$

where we have dropped constants such as factors of 2 or factors of a/L. The condition above also ensures that the correction to the unperturbed eigenfunction is also small.

(c) The parity of the the nth unperturbed energy level is $-(-1)^n$, corresponding to the behavior

$$\psi_n(-x) = -(-1)^n \psi_n(x) \,,$$

which follows from eq. (9). Noting that the unperturbed Hamiltonian and the perturbation $H^{(1)}$ are both even functions under $x \longrightarrow -x$, it follows that both the unperturbed and the exact Hamiltonians commute with the parity operator. Hence the exact energy eigenfunctions must have definite parity. In particular, if the unperturbed energy eigenfunction is odd under parity, then the perturbed wave function will also be odd under parity. This is indeed the case for the $n = 2$ energy eigenstate, as the explicit results of part (a) demonstrate.

5. Consider the Hamiltonian for positronium in the presence of a uniform external magnetic field, given in problem 2 above. Assume that the magnetic field points in the z-direction.

(a) Treating the magnetic field as a perturbation, compute the energy eigenvalues to second order in B and the energy eigenstates to first order in B. Sketch the energy levels as a function of B.

We take $\vec{\boldsymbol{B}} = B\hat{\boldsymbol{z}}$. The unperturbed Hamiltonian is given by

$$H^{(0)} = A\left[I - \frac{2}{\hbar^2}\left(\vec{\boldsymbol{S}}^{\,2} - \vec{\boldsymbol{S}}_{\boldsymbol{1}}^{\,2} - \vec{\boldsymbol{S}}_{\boldsymbol{2}}^{\,2}\right)\right] \,,$$

and the perturbation is given by

$$H^{(1)} = \frac{eB}{m}\left(S_{1z} - S_{2z}\right) \,.$$

As shown in problem 2, the unperturbed eigenstates are given by $|s\,,\, m_s\rangle$ with $s = 1$ for the ${}^3S_1$ triplet states and $s = 0$ for the ${}^1S_0$ singlet state.

First, consider the first-order energy shifts. For the ${}^1S_0$ singlet state,

$$E^{(1)}_{|0,0\rangle} = \frac{eB}{m}\,\langle 0\,,\,0|\,S_{1z} - S_{2z}\,|0\,,\,0\rangle \,.$$

To evaluate this, we convert from the total spin basis to the product basis. Recall that:

$$|0\,,\,0\rangle = \frac{1}{\sqrt{2}}\big[|\uparrow\,\downarrow\rangle - |\downarrow\,\uparrow\rangle\big]\,, \tag{10}$$

$$|1\,,\,0\rangle = \frac{1}{\sqrt{2}}\big[|\uparrow\,\downarrow\rangle + |\downarrow\,\uparrow\rangle\big]\,. \tag{11}$$

Then,

$$\begin{aligned} H^{(1)}\,|0\,,\,0\rangle &= \frac{eB}{\sqrt{2}\,m}\Big(S_{1z}\big[|\uparrow\,\downarrow\rangle - |\downarrow\,\uparrow\rangle\big] - S_{2z}\big[|\uparrow\,\downarrow\rangle - |\downarrow\,\uparrow\rangle\big]\Big) \\ &= \frac{e\hbar B}{\sqrt{2}\,m}\big[|\uparrow\,\downarrow\rangle + |\downarrow\,\uparrow\rangle\big] = \frac{e\hbar B}{m}\,|1\,,\,0\rangle\ . \end{aligned} \tag{12}$$

Since $|0\,,\,0\rangle$ and $|1\,,\,0\rangle$ are orthogonal states, it follows that $E^{(1)}_{|0,0\rangle} = 0$.

Next, consider the ${}^3S_1$ triplet states. These are three degenerate states with respect to $H^{(0)}$, so we must use degenerate perturbation theory. Thus, we shall evaluate the matrix

$$W_{m'_s,m_s} \equiv \langle 1\,,\,m'_s|\,H^{(1)}\,|1\,,\,m_s\rangle\ ,$$

which is a 3×3 matrix. To evaluate these matrix elements, we again rewrite the unperturbed eigenstates in terms of the product basis, using eq. (11) and

$$|1\,,\,1\rangle = |\uparrow\,\uparrow\rangle\ , \qquad\qquad |1\,,\,-1\rangle = |\downarrow\,\downarrow\rangle\ .$$

We compute:

$$\begin{aligned} H^{(1)}\,|1\,,\,1\rangle &= \frac{eB}{m}\,(S_{1z} - S_{2z})\,|\uparrow\,\uparrow\rangle = 0\,, \\ H^{(1)}\,|1\,,\,-1\rangle &= \frac{eB}{m}\,(S_{1z} - S_{2z})\,|\downarrow\,\downarrow\rangle = 0\,, \end{aligned}$$

and

$$\begin{aligned} H^{(1)}\,|1\,,\,0\rangle &= \frac{eB}{\sqrt{2}\,m}\Big(S_{1z}\big[|\uparrow\,\downarrow\rangle + |\downarrow\,\uparrow\rangle\big] - S_{2z}\big[|\uparrow\,\downarrow\rangle + |\downarrow\,\uparrow\rangle\big]\Big) \\ &= \frac{e\hbar B}{\sqrt{2}\,m}\big[|\uparrow\,\downarrow\rangle - |\downarrow\,\uparrow\rangle\big] = \frac{e\hbar B}{m}\,|0\,,\,0\rangle\ . \end{aligned}$$

Since the $|s\,,\,m_s\rangle$ states are orthonormal, it follows that

$$W_{m'_s,m_s} = 0\,, \qquad \text{for all}\ \ m_s\,,\,m_{s'} = -1\,,\,0\,,\,+1\,.$$

Thus, we have proven that all first-order energy shifts vanish.

Next, we consider the perturbed energy eigenstates at first order in the perturbation expansion. In class, we derived:

$$\left|n^{(1)}\right\rangle = \left|n^{(0)}\right\rangle + \sum_{m\neq n} \frac{\left|m^{(0)}\right\rangle \left\langle m^{(0)}\right| H^{(1)} \left|n^{(0)}\right\rangle}{E_n^{(0)} - E_m^{(0)}}\,, \tag{13}$$

where we *exclude* the degenerate states from the sum. Since $H^{(1)}\,|1\,,\,1\rangle = 0$ and $H^{(1)}\,|1\,,\,-1\rangle = 0$, it follows that there is no first order shift in the wave functions for $|1\,,\,1\rangle$ and $|1\,,\,-1\rangle$. On the other hand, there are first-order shifts in the wave functions for $|1\,,\,0\rangle$ and $|0\,,\,0\rangle$. Using eq. (13), it follows that

$$\left|\psi^{(1)}\right\rangle_{|1,0\rangle} = |1\,,\,0\rangle + \frac{|0\,,\,0\rangle \langle 0\,,\,0|\, H^{(1)}\,|1\,,\,0\rangle}{0-4A}\,,$$

$$\left|\psi^{(1)}\right\rangle_{|0,0\rangle} = |0\,,\,0\rangle + \frac{|1\,,\,0\rangle \langle 1\,,\,0|\, H^{(1)}\,|0\,,\,0\rangle}{4A-0}\,,$$

where we have used the unperturbed energies obtained in eq. (8). Evaluating these expressions using results obtained above, one finds:

$$\left|\psi^{(1)}\right\rangle_{|1,0\rangle} = |1\,,\,0\rangle - \frac{e\hbar B}{4Am}\,|0\,,\,0\rangle\ , \tag{14}$$

$$\left|\psi^{(1)}\right\rangle_{|0,0\rangle} = |0\,,\,0\rangle + \frac{e\hbar B}{4Am}\,|1\,,\,0\rangle\ . \tag{15}$$

The second order energy shifts can now be determined using

$$E^{(2)} = \left\langle n^{(0)}\right| H^{(1)} \left|n^{(1)}\right\rangle\ . \tag{16}$$

Due to $H^{(1)}\,|1\,,\,1\rangle = 0$ and $H^{(1)}\,|1\,,\,-1\rangle = 0$, it follows that there are no second-order energy shifts for $|1\,,\,1\rangle$ and $|1\,,\,-1\rangle$. On the other hand, there are second-order energy shifts for $|1\,,\,0\rangle$ and $|0\,,\,0\rangle$. Using eq. (16), one finds:

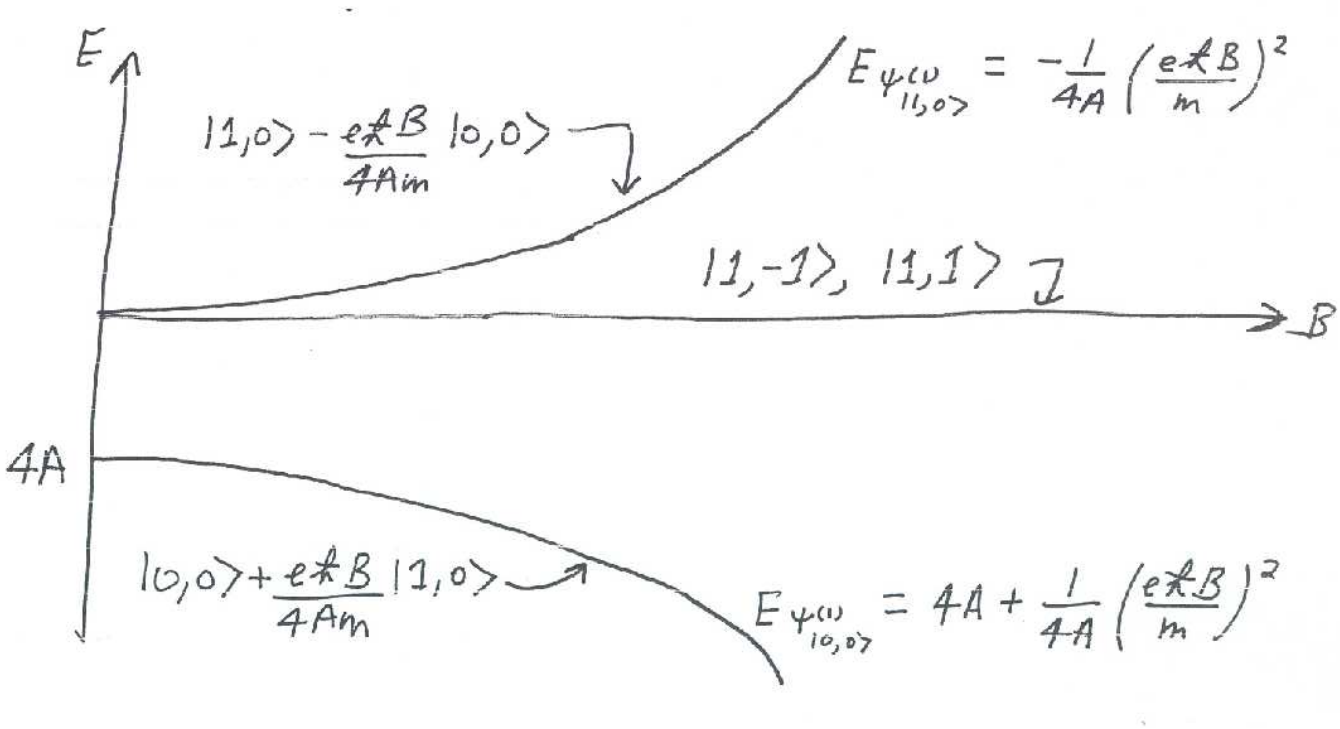
$$E^{(2)}_{|1,0\rangle} = \left\langle 1\,,\,0\right| H^{(1)} \left|\psi^{(1)}_{|1,0\rangle}\right\rangle = -\frac{e\hbar B}{4Am}\,\langle 1\,,\,0|\, H^{(1)}\,|0\,,\,0\rangle = -\frac{1}{4A}\left(\frac{e\hbar B}{m}\right)^2\ ,$$

$$E^{(2)}_{|0,0\rangle} = \left\langle 0\,,\,0\right| H^{(1)} \left|\psi^{(1)}_{|0,0\rangle}\right\rangle = \frac{e\hbar B}{4Am}\,\langle 0\,,\,0|\, H^{(1)}\,|1\,,\,0\rangle = \frac{1}{4A}\left(\frac{e\hbar B}{m}\right)^2\ .$$

The results obtained above are summarized in the following table:

$\underline{\text{state}}$	$\underline{\text{energy}}$
$\vphantom{\frac{1}{1}}\|1\,,\,1\rangle$	0
$\vphantom{\frac{1}{1}}\|1\,,\,0\rangle - \frac{e\hbar B}{4Am}\,\|0\,,\,0\rangle$	$-\frac{1}{4A}\left(\frac{e\hbar B}{m}\right)^2$
$\vphantom{\frac{1}{1}}\|1\,,\,-1\rangle$	0
$\vphantom{\frac{1}{1}}\|0\,,\,0\rangle + \frac{e\hbar B}{4Am}\,\|1\,,\,0\rangle$	$4A + \frac{1}{4A}\left(\frac{e\hbar B}{m}\right)^2$

where $A < 0$ as shown in problem 2(b). A sketch of the energy levels as a function of B is shown below.



REMARK: Since the degeneracy was not resolved at first order, one might worry that we have not yet identified the correct unperturbed degenerate eigenstates. In class, I indicated that to resolve the degeneracy at second order, one should solve the eigenvalue problem for the matrix $W^{(2)}$, which is defined by:

$$W^{(2)} = \sum_{k \neq n_i} \frac{\left\langle n_j^{(0)} \right| H^{(1)} \left| n_k^{(0)} \right\rangle \left\langle n_k^{(0)} \right| H^{(1)} \left| n_i^{(0)} \right\rangle}{E_{n^{(0)}} - E_{k^{(0)}}} \,,$$

where $\left| n_i^{(0)} \right\rangle$ are the degenerate states. Applying this result to the present problem, the sum over k consists of a sum over one unperturbed state, $|0\,,\,0\rangle$, which is not degenerate with the set of degenerate states $|1,\,,\,m_s\rangle$, $m_s = -1\,,\,0\,,\,+1$. Thus, the 3×3 matrix $W^{(2)}$ is given by:

$$W^{(2)}_{ji} = \frac{\left\langle n_j^{(0)} \right| H^{(1)} \left| 0\,,\,0 \right\rangle \left\langle 0\,,\,0 \right| H^{(1)} \left| n_i^{(0)} \right\rangle}{0 - 4A} = -\frac{1}{4A}\left(\frac{e\hbar B}{m}\right)^2 \left\langle n_j^{(0)} \right| \left. 1\,,\,0 \right\rangle \left\langle 1\,,\,0 \right| \left. n_i^{(0)} \right\rangle \,,$$

after using $H^{(1)}\,|0\,,\,0\rangle = (e\hbar B/m)\,|1\,,\,0\rangle$ obtained in eq. (12). Since the states $|1\,,\,m_s\rangle$, $m_s = -1\,,\,0\,,\,+1$ are orthonormal, it follows that $W^{(2)}$ is a diagonal

matrix in the total spin basis. Thus, the triplet states of the total spin basis are the correct unperturbed degenerate eigenstates. Moreover, the eigenvalues of $W^{(2)}$ are the correct second-order energy shifts—two zero energy eigenvalues corresponding to $|1\,,\,1\rangle$ and $|1\,,\,-1\rangle$, and a third energy eigenvalue given by $-[1/(4A)](e\hbar B/m)^2$. The corresponding energy eigenstate is also correctly computed in eq. (14), as we have employed the correct unperturbed degenerate eigenstates.

(b) Repeat the calculation of part (a), but now solve the problem exactly. Expand out your solutions in a power series in B, and verify that the results of part (a) are indeed correct.

This problem can be solved exactly by diagonalizing the full 4×4 matrix Hamiltonian,

$$\langle s'\,,\,m'_s|\,H^{(1)}\,|s\,,\,m_s\rangle\ ,$$

where

$$|s\,,\,m_s\rangle = \big\{|1\,,\,1\rangle\ ,\ |1\,,\,-1\rangle\ ,\ |1\,,\,0\rangle\ ,\ |0\,,\,0\rangle\big\} \tag{17}$$

indicates a convenient ordering of the entries in the rows and columns of the matrix representation of H. In fact, we have already computed all the matrix elements of H in part (a) of this problem. For example,

$$\begin{aligned} H\,|1\,,\,1\rangle &= (H^{(0)} + H^{(1)})\,|1\,,\,1\rangle = 0\,,\\ H\,|1\,,\,-1\rangle &= (H^{(0)} + H^{(1)})\,|1\,,\,-1\rangle = 0\,. \end{aligned}$$

Using results already obtained in problem 2 and in part (a) of this problem, the 4×4 matrix H with respect to the basis of eq. (17) is given by:

$$\langle s'\,,\,m'_s|\,H^{(1)}\,|s\,,\,m_s\rangle = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \dfrac{e\hbar B}{m} \\ 0 & 0 & \dfrac{e\hbar B}{m} & 4A \end{pmatrix}\ .$$

This matrix is easy to diagonalize. All we have to do is focus on the lower 2×2 block, i.e. the subspace spanned by $|1\,,\,0\rangle$ and $|0\,,\,0\rangle$,

$$\begin{pmatrix} 0 & \dfrac{e\hbar B}{m} \\ \dfrac{e\hbar B}{m} & 4A \end{pmatrix}\ .$$

The eigenvalues of this matrix are obtained by solving:

$$-E(4A - E) - \left(\frac{e\hbar B}{m}\right)^2 = 0\,.$$

The solutions to this quadratic equation are denoted by $E_\pm$, where

$$E_\pm = 2A \pm \sqrt{4A^2 + \left(\frac{e\hbar B}{m}\right)^2}\,. \tag{18}$$

To check that this reproduces the perturbative computation of part (a), we expand eq. (18) in a power series about $B = 0$. First rewrite:

$$E_\pm = 2A \mp 2A\left[1 + \frac{1}{4A^2}\left(\frac{e\hbar B}{m}\right)^2\right]^{1/2}\,.$$

Noting that $A < 0$, it follows that $\sqrt{A^2} = -A$ and so

$$\begin{aligned} E_\pm &\simeq 2A \mp 2A\left[1 + \frac{1}{8A^2}\left(\frac{e\hbar B}{m}\right)^2\right] \\ &= \begin{cases} -\dfrac{1}{4A}\left(\dfrac{e\hbar B}{m}\right)^2\,, & \text{for the state } \left|\psi^{(1)}_{|1,0\rangle}\right\rangle\,, \\ 4A + \dfrac{1}{4A}\left(\dfrac{e\hbar B}{m}\right)^2\,, & \text{for the state } \left|\psi^{(1)}_{|1,0\rangle}\right\rangle\,, \end{cases} \end{aligned} \tag{19}$$

in agreement with the results obtained in part (a).

To obtain the exact energy eigenfunction corresponding to the first eigenvalue E_+, we solve:

$$\begin{pmatrix} 0 & \dfrac{e\hbar B}{m} \\ \dfrac{e\hbar B}{m} & 4A \end{pmatrix} \begin{pmatrix} \cos\theta \\ \\ \sin\theta \end{pmatrix} = \left[2A + \sqrt{4A^2 + \left(\frac{e\hbar B}{m}\right)^2}\right] \begin{pmatrix} \cos\theta \\ \\ \sin\theta \end{pmatrix}\,, \tag{20}$$

since $\begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$ is the most general eigenvector of a real symmetric matrix that is normalized to unity. (Without loss of generality, one can take the energy eigenfunctions to be real.) Eq. (20) yields

$$\frac{e\hbar B}{m}\sin\theta = \left[2A + \sqrt{4A^2 + \left(\frac{e\hbar B}{m}\right)^2}\right]\cos\theta\,.$$

It is convenient to solve for $\tan\theta = \sin\theta/\cos\theta$. One then obtains:

$$\tan\theta = \frac{m}{e\hbar B}\left[2A + \sqrt{4A^2 + \left(\frac{e\hbar B}{m}\right)^2}\right]\,.$$

Using the identities,

$$\sin^2\theta = \frac{\tan^2\theta}{1+\tan^2\theta}\,, \qquad\qquad \cos^2\theta = \frac{1}{1+\tan^2\theta}\,,$$

one can compute:

$$\sin^2\theta = \frac{2A + \sqrt{4A^2 + \left(\dfrac{e\hbar B}{m}\right)^2}}{2\sqrt{4A^2 + \left(\dfrac{e\hbar B}{m}\right)^2}}\,,$$

$$\cos^2\theta = \frac{-2A + \sqrt{4A^2 + \left(\dfrac{e\hbar B}{m}\right)^2}}{2\sqrt{4A^2 + \left(\dfrac{e\hbar B}{m}\right)^2}}\,,$$

where we have used $\cos^2\theta = 1 - \sin^2\theta$. The above formulae look simpler when expressed in terms of the energy eigenvalues determined above. Using the results of eq. (18) and noting that:

$$E_+ - E_- = 2\sqrt{4A^2 + \left(\frac{e\hbar B}{m}\right)^2}\,,$$

it then follows that:

$$\sin^2\theta = \frac{E_+}{E_+ - E_-}\,, \qquad\qquad \cos^2\theta = \frac{-E_-}{E_+ - E_-}\,. \tag{21}$$

Since $A < 0$, one sees that $E_+ > 0$ and $E_- < 0$, in which case the above results are consistent with a real angle θ that can be chosen to lie in the range $0 \leq \theta \leq \pi/2$.

Thus, the eigenstate corresponding to the eigenvalue E_+ is given by:

$$\left(\frac{-E_-}{E_+ - E_-}\right)^{1/2} |1\,,\,0\rangle + \left(\frac{E_+}{E_+ - E_-}\right)^{1/2} |0\,,\,0\rangle\ .$$

The eigenstate corresponding to the eigenvalue E_- must be orthogonal to the eigenstate obtained above, and is thus given by:

$$-\left(\frac{E_+}{E_+ - E_-}\right)^{1/2} |1\,,\,0\rangle + \left(\frac{-E_-}{E_+ - E_-}\right)^{1/2} |0\,,\,0\rangle\ .$$

To complete the diagonalization of H, we note that the other two energy eigenvalues and eigenstates are not shifted by the perturbation due to the zeros in the matrix. That is, the other two eigenstates are $|1\,,\,1\rangle$ and $|1\,,\,-1\rangle$ with corresponding zero eigenvalues, to all orders in perturbation theory.

To summarize, the exact energy eigenstates and eigenvalues are given in the following table:

state	energy
$\|1\,,\,1\rangle$	0
$\left(\frac{-E_-}{E_+-E_-}\right)^{1/2}\|1\,,\,0\rangle + \left(\frac{E_+}{E_+-E_-}\right)^{1/2}\|0\,,\,0\rangle$	E_+
$\|1\,,\,-1\rangle$	0
$-\left(\frac{E_+}{E_+-E_-}\right)^{1/2}\|1\,,\,0\rangle + \left(\frac{-E_-}{E_+-E_-}\right)^{1/2}\|0\,,\,0\rangle$	E_-

where

$$E_\pm \equiv 2A \pm \sqrt{4A^2 + \left(\frac{e\hbar B}{m}\right)^2}\,.$$

As a final check, one can expand these results in a power series about $B = 0$ and show that one obtains the energy eigenfunctions at first order that match the results obtained in part(a). Using eqs. (19) and (21), one finds:

$$\sin^2\theta = \frac{E_+}{E_+ - E_-} \simeq \frac{-\dfrac{1}{4A}\left(\dfrac{e\hbar B}{m}\right)^2}{-4A - \dfrac{1}{2A}\left(\dfrac{e\hbar B}{m}\right)^2} = \frac{1}{16A^2}\left(\frac{e\hbar B}{m}\right)^2 + \mathcal{O}(B^4)\,,$$

Since $0 \leq \theta \leq \pi/2$ by convention (and $A < 0$), it follows that

$$\sin\theta \simeq -\frac{1}{4A}\left(\frac{e\hbar B}{m}\right) + \mathcal{O}(B^3)\,.$$

Finally,

$$\cos^2\theta = 1 - \sin^2\theta = 1 - \mathcal{O}(B^2)\,,$$

and therefore

$$\cos\theta = 1 - \mathcal{O}(B^2)\,.$$

That is, we identify:

$$\left|\psi^{(1)}_{|1,0\rangle}\right\rangle = \cos\theta\,|1\,,\,0\rangle + \sin\theta\,|0\,,\,0\rangle \simeq |1\,,\,0\rangle - \left(\frac{e\hbar B}{4Am}\right)|0\,,\,0\rangle\ ,$$

$$\left|\psi^{(1)}_{|0,0\rangle}\right\rangle = -\sin\theta\,|1\,,\,0\rangle + \cos\theta\,|0\,,\,0\rangle \simeq |0\,,\,0\rangle + \left(\frac{e\hbar B}{4Am}\right)|1\,,\,0\rangle\ ,$$

which reproduces the results obtained in part (a) by the first-order perturbation theory computation.