Columbia University
Department of Physics
QUALIFYING EXAMINATION

Wednesday, January 11, 2017
11:00AM to 1:00PM
Modern Physics
Section 3. Quantum Mechanics

Two hours are permitted for the completion of this section of the examination. Choose
4 problems out of the 5 included in this section. (You will not earn extra credit by doing an
additional problem). Apportion your time carefully.

Use separate answer booklet(s) for each question. Clearly mark on the answer booklet(s)
which question you are answering (e.g., Section 3 (QM), Question 2, etc.).

Do **NOT** write your name on your answer booklets. Instead, clearly indicate your **Exam
Letter Code**.

You may refer to the single handwritten note sheet on $8\frac{1}{2}$" $\times$ 11" paper (double-sided) you
have prepared on Modern Physics. The note sheet cannot leave the exam room once the
exam has begun. This note sheet must be handed in at the end of today's exam. Please
include your Exam Letter Code on your note sheet. No other extraneous papers or books
are permitted.

Simple calculators are permitted. However, the use of calculators for storing and/or recov-
ering formulae or constants is NOT permitted.

Questions should be directed to the proctor.

Good Luck!

1. Let a, $a^\dagger$ the standard harmonic oscillator creation and annihilation operators, $[a, a^\dagger] = 1$. Consider a Hamiltonian which in suitable units takes the form

$$H = a^\dagger a + \lambda(a + a^\dagger),\tag{1}$$

where λ is a real constant. This can be viewed as a perturbation of the standard harmonic oscillator hamiltonian $H^{(0)} = a^\dagger a$.

(a) Compute the ground state energy of H to second order in perturbation theory in λ.

(b) Find the exact spectrum of H. (You can do this by judiciously defining new creation and annihilation operators b and $b^\dagger$, related to the original a and $a^\dagger$ by a constant shift, and noticing this maps the hamiltonian to one for which the spectrum is obvious.)

(c) Assuming that in suitable units, a is related to the position operator x and momentum operator p by $a = x + ip$, find the ground state wave function of H.

2. _____

The following integrals may be useful for this problem:

$$\int_0^L \sin \tfrac{m\pi x}{L} \, \sin \tfrac{n\pi x}{L} \, dx = \begin{cases} \tfrac{L}{2} & \text{if } m = n \\ 0 & \text{if } m \neq n \end{cases} \tag{2}$$

$$\int_0^L \sin \tfrac{m\pi x}{L} \, \cos \tfrac{n\pi x}{L} \, dx = \begin{cases} \tfrac{2L}{\pi} \tfrac{m}{(m^2-n^2)} & \text{if } m + n \text{ is odd} \\ 0 & \text{if } m + n \text{ is even} \end{cases} \tag{3}$$

Consider a nonrelativistic particle of mass m confined in an infinitely deep square potential well $V(x)$, that is to say $V(x) = 0$ for $0 < x < L$ and $V(x) = \infty$ for $x < 0$ and for $x > L$.

(a) Find the values of E_1, E_2 such that the wave function

$$\psi(x,t) = A \sin \tfrac{\pi x}{L} \, e^{-iE_1 t/\hbar} + B \sin \tfrac{2\pi x}{L} \, e^{-iE_2 t/\hbar} \qquad (0 < x < L) \tag{4}$$

satisfies the time-dependent Schrödinger equation.

(b) Show that the wave function has unit norm for any (A, B) satisfying $|A|^2 + |B|^2 = \tfrac{2}{L}$.

(c) Find the expectation values of the following physical quantities:

  1. Energy E, for arbitrary (A, B).
  2. Position x, assuming $A = 0$.
  3. Momentum p_x, assuming $A = B$.

You may like to use symmetry arguments and/or the integrals (2)-(3) to compute these.

3. A non-relativistic particle of mass m moves in one dimension, subject to a potential energy function $V(x)$ which is the sum of three evenly-spaced, attractive delta functions:

$$V(x) = -V_0\, a\big(\delta(x+a) + \delta(x) + \delta(x-a)\big) \quad \text{where} \quad V_0, a > 0 \tag{5}$$

This problem studies the quantum bound states of this potential.

(a) Calculate the discontinuity in the first derivative of the wavefunction at $x = -a, 0$ and a.

(b) Without solving the full problem, consider the possible number and location of nodes in bound state wavefunctions for the system.

   1. How many nodes are possible in the region $x > a$?
   2. How many nodes are possible in the region $0 < x < a$?
   3. Can there be a node at $x = a$?
   4. Can there be a node at $x = 0$?

(c) If V_0 is large enough, the system will have both symmetric ($\psi(-x) = \psi(x)$) and anti-symmetric bound states ($\psi(-x) = -\psi(x)$). Without solving the full problem, sketch qualitatively the symmetric and anti-symmetric bound states in this case.

(d) For the anti-symmetric bound states, derive a transcendental equation that determines the bound state energy. You do not need to solve the equation.

4. Consider a two state system with kets $|0\rangle$ and $|1\rangle$ defining a set which is assumed to be orthonormal and complete. The Hamiltonian of the system is

$$\hat{H} = \hbar\omega\hat{a}^\dagger\hat{a} \tag{6}$$

where the operators $\hat{a}$ and $\hat{a}^\dagger$ are defined by

$$\hat{a}^\dagger|0\rangle = |1\rangle, \quad \hat{a}|1\rangle = |0\rangle, \quad \hat{a}|0\rangle = \hat{a}^\dagger|1\rangle = 0 \tag{7}$$

(a) Find the eigenvalues of $\hat{H}$.

(b) Write down the Dirac (bra-ket) representation of the operators $\hat{H}$, $\hat{a}$ and $\hat{a}^\dagger$.

(c) What are the anti-commutators of the operators $\hat{a}$ and $\hat{a}^\dagger$?

5. We consider a system of two spins, spin 1 and spin 2. The system can be described in the basis $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$, where the first entry denotes the state of spin 1 and the second entry the state of spin 2. The spins interact via the Hamiltonian:

$$\hat{H} = E_0 + \frac{A}{4}\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 = E_0 + \frac{A}{4}(\hat{\sigma}_{1x}\hat{\sigma}_{2x} + \hat{\sigma}_{1y}\hat{\sigma}_{2y} + \hat{\sigma}_{1z}\hat{\sigma}_{2z}) \tag{8}$$

A is a constant denoting the strength of the spin-spin coupling and E_0 is an arbitrary energy offset. The matrices σ_{ix}, σ_{iy}, and σ_{iz} are the typical Pauli matrices $(i = 1, 2)$.

We assume that, at time $t = 0$, the spin system is in state $|\psi(0)\rangle = \alpha |\uparrow\uparrow\rangle + \beta |\uparrow\downarrow\rangle$ with the normalization $|\alpha|^2 + |\beta|^2 = 1$.

(a) Write the Hamiltonian $\hat{H}$ in matrix representation in the above basis.

(b) Determine the eigenbasis of $\hat{H}$.

(c) Express the state $|\psi(0)\rangle$ in terms of the eigenbasis of $\hat{H}$.

(d) Calculate $|\psi(t)\rangle$ at a later time.

2017 Quals — section 3 — Denef — solution

December 15, 2016

Let a, $a^\dagger$ the standard harmonic oscillator creation and annihilation operators, $[a, a^\dagger] = 1$. Consider a Hamiltonian which in suitable units takes the form

$$H = a^\dagger a + \lambda(a + a^\dagger),\tag{1}$$

where λ is a real constant. This can be viewed as a perturbation of the standard harmonic oscillator hamiltonian $H^{(0)} = a^\dagger a$.

(a) Compute the ground state energy of H to second order in perturbation theory in λ.

Denote the unperturbed ground state of $H^{(0)}$ by $|0\rangle$. Then $a|0\rangle = 0$. To first order in perturbation theory, the ground state energy is $E_0^{(1)} = \langle 0|H|0\rangle = 0$. To second order in perturbation theory, the ground state energy is

$$E_0^{(2)} = \lambda^2 \sum_{n \neq 0} \frac{|\langle n|a + a^\dagger|0\rangle|^2}{E_0^{(0)} - E_n^{(0)}} = \lambda^2 \frac{|\langle 1|a^\dagger|0\rangle|^2}{0 - 1} = -\lambda^2.\tag{2}$$

(b) Find the exact spectrum of H. (You can do this by judiciously defining new creation and annihilation operators b and $b^\dagger$, related to the original a and $a^\dagger$ by a constant shift, and noticing this maps the hamiltonian to one for which the spectrum is obvious.)

If we define $b = a + \lambda$, $b^\dagger = a^\dagger + \lambda$, then $[b, b^\dagger] = 1$ and $H = b^\dagger b - \lambda^2$. So this is the hamiltonian of a harmonic oscillator with creation and annihilation operators $b, b^\dagger$, with a constant energy shift $-\lambda^2$. The exact spectrum is therefore

$$E_n = n - \lambda^2, \qquad n = 0, 1, 2, \dots.\tag{3}$$

Note that this is in agreement with the second order perturbation theory result obtained earlier.

(c) *Assuming that in suitable units, a is related to the position operator x and momentum operator p by $a = x + ip$, find the ground state wave function of H.*

The ground state wave function $\psi_0(x)$ satisfies $b\,\psi_0 = 0$, that is to say $(\lambda + x + \partial_x)\psi_0(x) = 0$. This is easily solved as

$$\psi_0(x) = A\,e^{-\frac{1}{2}(x+\lambda)^2}\,, \tag{4}$$

where A is a suitable normalization constant $\left(A = \frac{1}{(2\pi)^{1/4}}\right)$.

2017 Quals — section 3 — Dodd (variant by FD): solution

December 15, 2016

The following integrals may be useful for this problem:

$$\int_0^L \sin \tfrac{m\pi x}{L} \, \sin \tfrac{n\pi x}{L} \, dx = \begin{cases} \tfrac{L}{2} & \textit{if } m = n \\ 0 & \textit{if } m \neq n \end{cases} \tag{1}$$

$$\int_0^L \sin \tfrac{m\pi x}{L} \, \cos \tfrac{n\pi x}{L} \, dx = \begin{cases} \tfrac{2L}{\pi} \tfrac{m}{(m^2 - n^2)} & \textit{if } m + n \textit{ is odd} \\ 0 & \textit{if } m + n \textit{ is even} \end{cases} \tag{2}$$

(a) *Find the values of E_1, E_2 such that the wave function*

$$\psi(x,t) = A \sin \tfrac{\pi x}{L} \, e^{-iE_1 t} + B \sin \tfrac{2\pi x}{L} \, e^{-iE_2 t} \qquad (0 < x < L) \tag{3}$$

satisfies the time-dependent Schrödinger equation.

The time dependent Schrödinger equation inside the potential well is

$$i\hbar \partial_t \psi = -\frac{\hbar^2}{2m} \partial_x^2 \psi \,. \tag{4}$$

Substituting the given form of $\psi(t, x)$ into this equation gives

$$E_1 \, A \sin \tfrac{\pi x}{L} \, e^{-iE_1 t/\hbar} + E_2 \, B \sin \tfrac{2\pi x}{L} \, e^{-iE_2 t/\hbar}$$
$$= \frac{\hbar^2 \pi^2}{2mL^2} A \sin \tfrac{\pi x}{L} \, e^{-iE_1 t/\hbar} + \frac{4\hbar^2 \pi^2}{2mL^2} B \sin \tfrac{2\pi x}{L} \, e^{-iE_2 t/\hbar} \,,$$

from which we read off

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2} \,, \qquad E_2 = \frac{4\hbar^2 \pi^2}{2mL^2} \,. \tag{5}$$

(b) *Show that the wave function has unit norm for any (A, B) satisfying $|A|^2 + |B|^2 = \frac{1}{2L}$.*

Using (1) we immediately get

$$\int_0^L dx\, \psi(t, x)^* \, \psi(t, x) = \frac{L}{2} \left(|A|^2 + |B|^2 \right) , \qquad (6)$$

so for the wave function to be unit normalized, we need $|A|^2 + |B|^2 = \frac{2}{L}$.

(c) *Find the expectation values of the following physical quantities:*

1. *Energy, for arbitrary (A, B).*

   Since the wave function is the superposition of two energy eigenstates with energies E_1 and E_2 and coefficients A and B, the expectation value of the energy E is

   $$\langle E \rangle = \frac{|A|^2 \, E_1 + |B|^2 \, E_2}{|A|^2 + |B|^2} = \frac{|A|^2 + 4\,|B|^2}{|A|^2 + |B|^2} \frac{\hbar^2 \pi^2}{2mL^2} . \qquad (7)$$

2. *Position, assuming $A = 0$.*

   The expectation value of the position is $\langle x \rangle = \int |\psi(x, t)|^2 \, x \, dx$. If $A = 0$, the wave function squared is symmetric under reflection about the midpoint $x = \frac{L}{2}$. Therefore $\langle x \rangle = \frac{L}{2}$.

3. *Momentum, assuming $A = B$.*

   If $A = B$, the normalized wave function is

   $$\psi(x, t) = \frac{1}{\sqrt{L}} \left(\sin \frac{\pi x}{L} e^{-iE_1 t} + \sin \frac{2\pi x}{L} e^{-iE_2 t} \right) \qquad (8)$$

   The expectation value of the momentum is then, using (2),

   $$\begin{aligned}
   \langle p_x \rangle &= \int_0^L \psi(x, t)^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi(x, t) \\
   &= \frac{i\hbar\pi}{L^2} \int_0^L \left(\sin \frac{\pi x}{L} \cos \frac{\pi x}{L} + 2 \sin \frac{\pi x}{L} \cos \frac{2\pi x}{L} e^{-i(E_2 - E_1)t/\hbar} \right. \\
   &\qquad \left. + \sin \frac{2\pi x}{L} \cos \frac{\pi x}{L} e^{i(E_2 - E_1)t/\hbar} + \sin \frac{2\pi x}{L} \cos \frac{2\pi x}{L} \right) dx \\
   &= \frac{i\hbar\pi}{L^2} \frac{2L}{\pi} \left(-\frac{2}{3} e^{-i(E_2 - E_1)t/\hbar} + \frac{2}{3} e^{i(E_2 - E_1)t/\hbar} \right) \\
   &= \frac{8\hbar}{3L} \sin\left((E_2 - E_1)t/\hbar \right) \\
   &= \frac{8\hbar}{3L} \sin\left(\frac{3\hbar\pi^2}{2mL^2} t \right) .
   \end{aligned} \qquad (9)$$

① $$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi = E\psi$$

Integrating across any of the delta functions gives

$$\frac{-\hbar^2}{2m} \left(\partial_x \psi \Big|_{x=y-\varepsilon} - \partial_x \psi \Big|_{x=y+\varepsilon} \right) - V_0 a \psi(y) = 0$$

for $y = -a, 0, a$

② Away from the delta functions, the eigenfunctions satisfy

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E\psi$$

For a bound state in a potential which goes to zero at $x = \infty$, we need $E < 0$ so the general solution is.

$$\psi(x) = A e^{Kx} + B e^{-Kx} \qquad K = \frac{\sqrt{-2mE}}{\hbar}$$

The only way this function can vanish is if A and B have opposite signs in which case there is a unique zero.

② ⓐ For $x > a$, $A = 0$, so the solution is normalizable. There are <u>no</u> zeros, since $Be^{-\kappa x}$ has no zeros.

ⓑ There can be zero or one node in $0 < x < a$.

ⓒ No node at $x = a$, since then ψ would have to vanish for $x > a$

ⓓ yes, there can be a node

③ The largest number of boundstates is three.
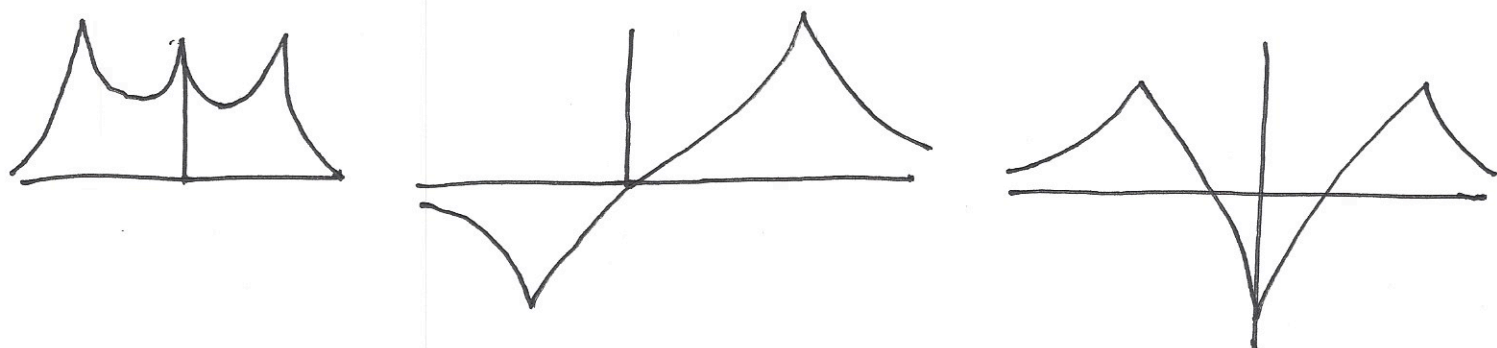
④ Bound state solution with $\psi(x) = -\psi(x)$ is

$$\psi(x) = \begin{cases} Ae^{-\kappa x} & a \leq x \\ B(e^{\kappa x} - e^{-\kappa x}) & 0 \leq x \leq a \end{cases}$$

~~cont~~ continuity

$$Ae^{-\kappa a} = Be^{\kappa a} - e^{-\kappa a}$$

④ – continued –

Derivative condition

$$k\left(B(e^{ka}+e^{-ka})+Ae^{-ka}\right)=\frac{-2m}{\hbar^2}aV_oAe^{-ka}$$

Eliminating A,

$$\frac{ka}{1-e^{-2ka}}=\frac{mV_oa^2}{\hbar^2}$$

2017 Quals Problem: Quantum Mechanics

Consider a two state system with kets $|0\rangle$ and $|1\rangle$ defining a set which is assumed to be orthonormal and complete. The Hamiltonian of the system is

$$\hat{H} = \hbar\omega\hat{a}^\dagger\hat{a}$$

where the operators $\hat{a}$ and $\hat{a}^\dagger$ are defined by

$$\hat{a}^\dagger|0\rangle = |1\rangle \,, \quad \hat{a}|1\rangle = |0\rangle \,, \quad \hat{a}|0\rangle = \hat{a}^\dagger|1\rangle = 0 \,.$$

a. Find the eigenvalues of $\hat{H}$.

b. Write down the Dirac (bra-ket) representation of the operators $\hat{H}$, $\hat{a}$ and $\hat{a}^\dagger$.

c. What are the anti-commutators of the operators $\hat{a}$ and $\hat{a}^\dagger$?

2017 Quals Problem: Quantum Mechanics
Solution

a.
$$\hat{H}|0\rangle = \hbar\omega\hat{a}^\dagger\hat{a}|0\rangle = 0 \quad \Rightarrow \quad E_0 = 0$$
$$\hat{H}|1\rangle = \hbar\omega\hat{a}^\dagger\hat{a}|1\rangle = \hbar\omega\hat{a}^\dagger|0\rangle = \hbar\omega|1\rangle \quad \Rightarrow \quad E_1 = \hbar\omega$$

b.
$$\hat{O} = \sum |n\rangle\langle n|\hat{O}|m\rangle\langle m|$$
$\hat{H}$ is diagonal: $\hat{H} = 0|0\rangle\langle 0| + \hbar\omega|1\rangle\langle 1| = \hbar\omega|1\rangle\langle 1|$
$$\hat{a} = |0\rangle\langle 0|\hat{a}|1\rangle\langle 1| = |0\rangle\langle 1|$$
$$\hat{a}^\dagger = |1\rangle\langle 1|\hat{a}^\dagger|0\rangle\langle 0| = |1\rangle\langle 0|$$

c.
$$\hat{a}\hat{a}^\dagger = |0\rangle\langle 1|1\rangle\langle 0| = |0\rangle\langle 0|$$
$$\hat{a}^\dagger\hat{a} = |1\rangle\langle 0|0\rangle\langle 1| = |1\rangle\langle 1|$$
$$\{\hat{a}, \hat{a}^\dagger\} = |0\rangle\langle 0| + |1\rangle\langle 1| = \mathbb{1}$$
Also $\{\hat{a}, \hat{a}\} = \{\hat{a}^\dagger, \hat{a}^\dagger\} = 0$

Problem Suggestion Quals 2017

Quantum Mechanics

Sebastian Will*

Columbia University

(Dated: November 18, 2016)

INTERACTING SPIN-$\frac{1}{2}$ SYSTEMS

We consider a system of two spins, spin 1 and spin 2. The system can be described in the basis $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$, where the first entry denotes the state of spin 1 and the second entry the state of spin 2. The spins interact via the Hamiltonian:

$$\hat{H} = E_0 + \frac{A}{4}\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2 = E_0 + \frac{A}{4}(\hat{\sigma}_{1x}\hat{\sigma}_{2x} + \hat{\sigma}_{1y}\hat{\sigma}_{2y} + \hat{\sigma}_{1z}\hat{\sigma}_{2z}).$$

A is a constant denoting the strength of the spin-spin coupling and E_0 is an arbitrary energy offset. The matrices σ_{ix}, σ_{iy}, and σ_{iz} are the typical Pauli matrices ($i = 1, 2$).

We assume that, at time $t = 0$, the spin system is in state $|\psi(0)\rangle = \alpha|\uparrow\uparrow\rangle + \beta|\uparrow\downarrow\rangle$ with the normalization $|\alpha|^2 + |\beta|^2 = 1$.

(a) Write the Hamiltonian $\hat{H}$ in matrix representation in the above basis. **8 mins**

(b) Determine the eigenbasis of $\hat{H}$. **8 mins**

(c) Express the state $|\psi(0)\rangle$ in terms of the eigenbasis of $\hat{H}$. **5 mins**

(d) Calculate $|\psi(t)\rangle$ at a later time. **3 mins**

Note: The problem can be simplified (or extended) in various ways if necessary. Let me know.

SOLUTION

(a) The action of $\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2$ on the basis states is:

$$\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2|\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle$$

$$\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2|\uparrow\downarrow\rangle = 2|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle$$

$$\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2|\downarrow\uparrow\rangle = 2|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$

$$\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2|\downarrow\downarrow\rangle = |\downarrow\downarrow\rangle.$$

Hence, the matrix representation is

$$\hat{H} = \begin{pmatrix} E_0 + A/4 & 0 & 0 & 0 \\ 0 & E_0 - A/4 & A/2 & 0 \\ 0 & A/2 & E_0 - A/4 & 0 \\ 0 & 0 & 0 & E_0 + A/4 \end{pmatrix}$$

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(b) The eigenbasis of $\hat{H}$ consists of the eigenstates of the total spin operators $\hat{S}^2$ and $\hat{S}_z$. The students do not need to know that to get full points. The triplet states $(S = 1)$:

$$|1, 1\rangle = |\uparrow\uparrow\rangle$$
$$|1, 0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$$
$$|1, -1\rangle = |\downarrow\downarrow\rangle$$

and the singlet state $(S = 0)$:

$$|0, 0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle).$$

(c) The representation in the eigenbasis is

$$|\psi(0)\rangle = \alpha|1, 1\rangle + \frac{\beta}{\sqrt{2}}(|1, 0\rangle + |0, 0\rangle).$$

(d) The eigenenergy of the triplet states is $E_0 + A/4$ and the eigenenergy of the singlet state is $E_0 - 3A/4$. Therefore the time evolution of $|\psi\rangle$ can be written as

$$|\psi(t)\rangle = e^{-iE_0t/\hbar}\left[e^{-iAt/(4\hbar)}\left(\alpha|1, 1\rangle + \frac{\beta}{\sqrt{2}}|1, 0\rangle\right) + \frac{\beta}{\sqrt{2}}e^{i3At/(4\hbar)}|0, 0\rangle\right].$$

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