Chapter 4 Problems and Solutions
J.J. Sakurai and Jim Napolitano
Modern Quantum Mechanics, 2nd edition
(Pearson, 2011)

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((**4-1**))

4.1 Calculate the *three lowest* energy levels, together with their degeneracies, for the following systems (assume equal-mass *distinguishable* particles).

(a) Three noninteracting spin $\frac{1}{2}$ particles in a box of length L.

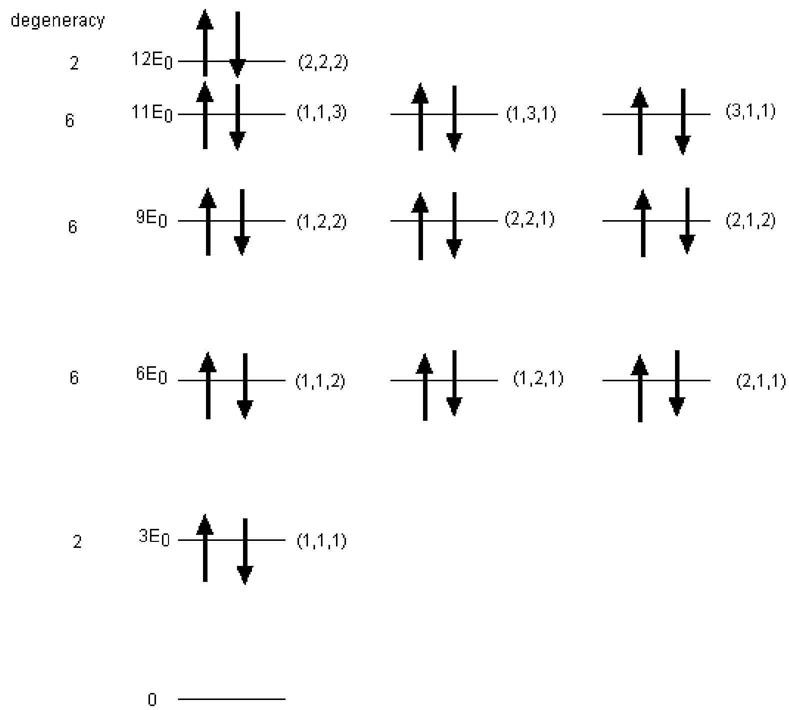
(b) Four noninteracting spin $\frac{1}{2}$ particles in a box of length L.

((**Solution**))
The energy is given by

$$E(n_x, n_y, n_z) = E_0(n_x{}^2 + n_y{}^2 + n_z{}^2)$$

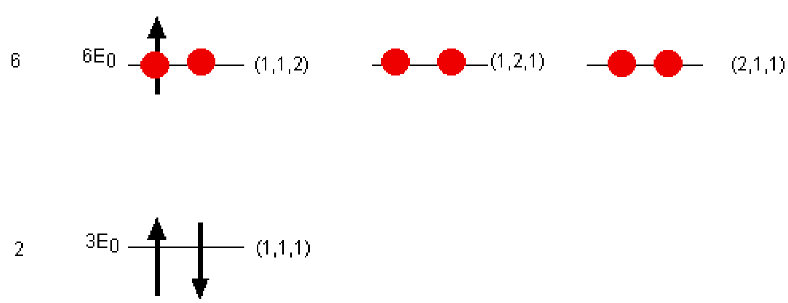
where $E_0 = \frac{\hbar^2}{2m}(\frac{\pi}{L})^2$, and n_x, n_y, n_z are positive integers.

We consider the Pauli principle.



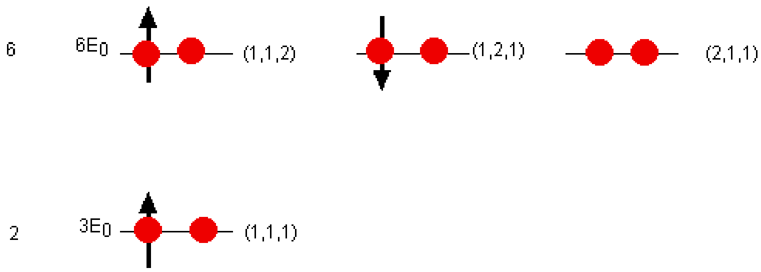
(a) 3 noninteracting spin 1/2 particles

<u>Ground state:</u> $E = 12\ E_0$



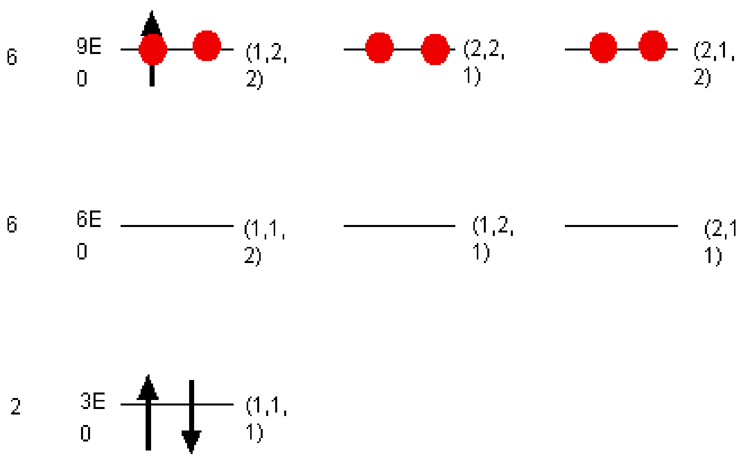
Energy = $3E_0 + 3E_0 + 6\ E_0 = 12\ E_0$
degeneracy $g_0 = {}_2C_2$ x ${}_6C_1 = 6$.

<u>First excited state (1)</u>: $E = 15\ E_0$



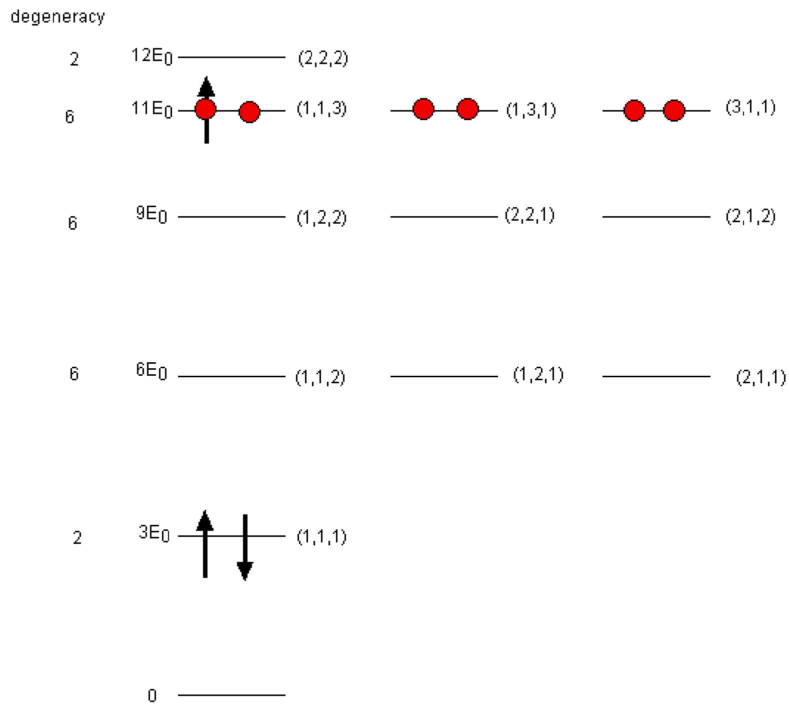
Energy = $3E_0 + 6E_0 + 6\ E_0 = 15\ E_0$
degeneracy $g_0 = {}_2C_1 \text{ x } {}_6C_2 = 15 \text{ x } 2 = 30$ states

First excited state (2):$E = 15\ E_0$



Energy = $3E_0 + 3E_0 + 9\ E_0 = 15\ E_0$
degeneracy $g_0 = {}_2C_2 \text{ x } {}_6C_1 = 1 \text{ x } 6 = 6$ states

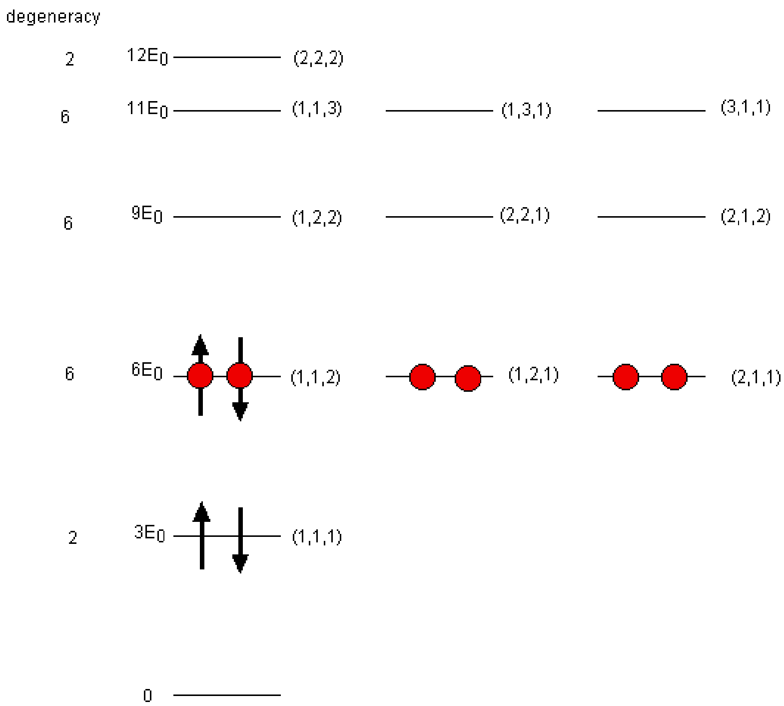
Second excited state: $E = 17\ E_0$



Energy = $3E_0 + 3E_0 + 11\ E_0 = 17\ E_0$
degeneracy $g_0 = {}_2C_2 \text{ x } {}_6C_1 = 1 \text{ x } 6 = 6$ states

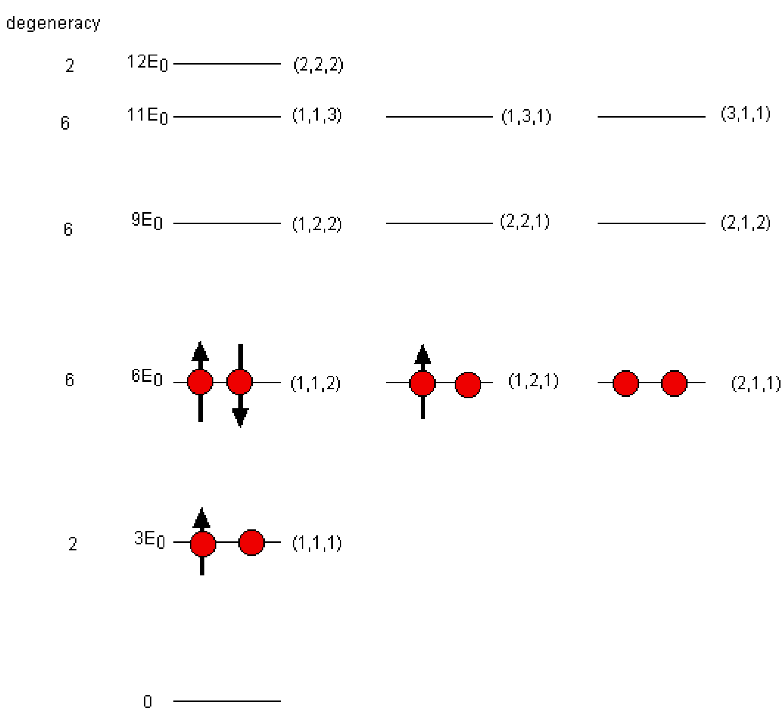
(b) Four noninteracting spin 1/2 particles

<u>Ground state</u>: $E = 18\ E_0$



Energy = $3E_0 + 3E_0 + 6E_0 + 6E_0 = 18E_0$
degeneracy $g_0 = {}_2C_2 \times {}_6C_2 = 1 \times 15 = 15$ states

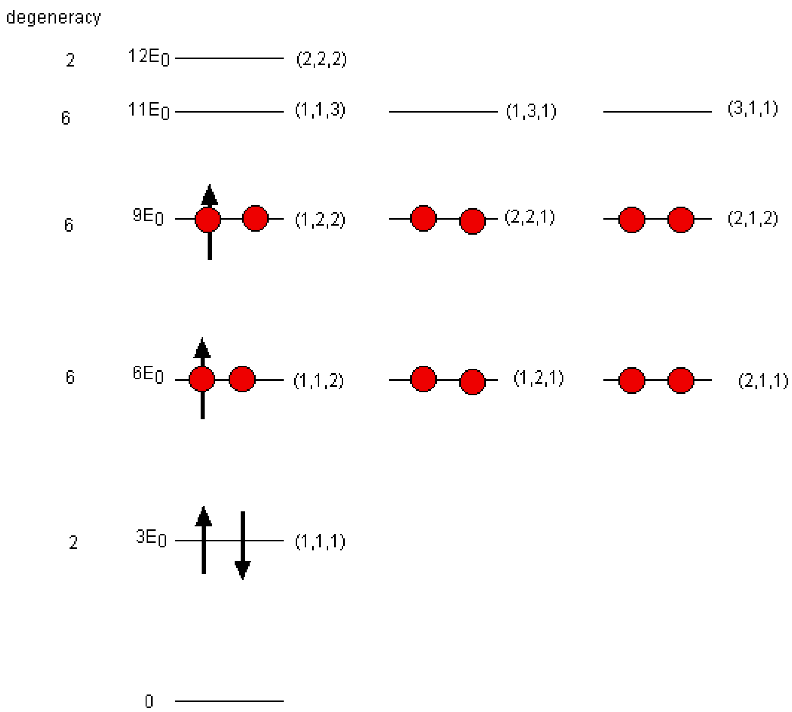
First excited state (1): $E = 21E_0$



Energy = $6E_0 + 6E_0 + 6E_0 + 3E_0 = 21E_0$

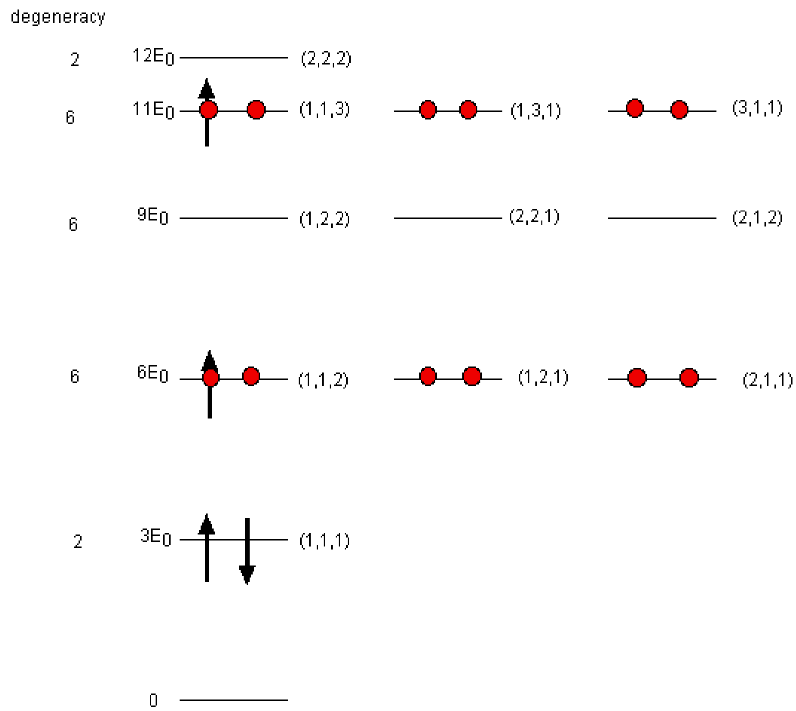
degeneracy $g_0 = {}_2C_1 \times {}_6C_3 = 40$ states

First excited state (2): $E = 21\ E_0$



Energy = $3\ E_0 + 3E_0 + 6\ E_0 + 9\ E_0 = 21\ E_0$
degeneracy $g_0 = {}_2C_2 \times {}_6C_1 \times {}_6C_1 = 36$ states

Second excited state: $E = 23\ E_0$



Energy = 3 E_0 + 3E_0 +6 E_0 + 11 E_0= 23 E_0
degeneracy $g_0 = {}_2C_2 \times {}_6C_1 \times {}_6C_1$ = 36 states

((**4-2**))

4.2 Let $\mathcal{T}_{\mathbf{d}}$ denote the translation operator (displacement vector **d**); let $\mathcal{D}(\hat{\mathbf{n}},\phi)$ denote the rotation operator ($\hat{\mathbf{n}}$ and ϕ are the axis and angle of rotation, respectively); and let π denote the parity operator. Which, if any, of the following pairs commute? Why?

(a) $\mathcal{T}_{\mathbf{d}}$ and $\mathcal{T}_{\mathbf{d}'}$ (**d** and **d**′ in different directions).

(b) $\mathcal{D}(\hat{\mathbf{n}},\phi)$ and $\mathcal{D}(\hat{\mathbf{n}}',\phi')$ ($\hat{\mathbf{n}}$ and $\hat{\mathbf{n}}'$ in different directions).

(c) $\mathcal{T}_{\mathbf{d}}$ and π.

(d) $\mathcal{D}(\hat{\mathbf{n}},\phi)$ and π.

((**Solution**))

(a)

$$\hat{T}_d = \exp\left(-\frac{i\hat{\boldsymbol{P}}\cdot\boldsymbol{d}}{\hbar}\right), \qquad \hat{T}_{d'} = \exp\left(-\frac{i\hat{\boldsymbol{P}}\cdot\boldsymbol{d}'}{\hbar}\right)$$

$$\hat{T}_d|\boldsymbol{r}\rangle = |\boldsymbol{r}+\boldsymbol{d}\rangle, \qquad \hat{T}_{d'}|\boldsymbol{r}\rangle = |\boldsymbol{r}+\boldsymbol{d}'\rangle$$

$$\hat{T}_d\hat{T}_{d'}|\boldsymbol{r}\rangle = \hat{T}_d|\boldsymbol{r}+\boldsymbol{d}'\rangle = |\boldsymbol{r}+\boldsymbol{d}+\boldsymbol{d}'\rangle$$

$$\hat{T}_{d'}\hat{T}_d|\boldsymbol{r}\rangle = \hat{T}_{d'}|\boldsymbol{r}+\boldsymbol{d}\rangle = |\boldsymbol{r}+\boldsymbol{d}+\boldsymbol{d}'\rangle$$

$$\hat{T}_d\hat{T}_{d'} = \hat{T}_{d'}\hat{T}_d$$

(b)

$$\hat{R}(\boldsymbol{n},\phi) = \exp\left(-\frac{i}{\hbar}\hat{\boldsymbol{J}}\cdot\boldsymbol{n}\phi\right), \;\; \hat{R}(\boldsymbol{n},\phi') = \exp\left(-\frac{i}{\hbar}\hat{\boldsymbol{J}}\cdot\boldsymbol{n}'\phi'\right)$$

$$\hat{R}(\boldsymbol{n}',\phi')|\boldsymbol{r}\rangle = |\Re_{\boldsymbol{n}'}(\phi')\boldsymbol{r}\rangle$$

$$\hat{R}(\boldsymbol{n},\phi)\hat{R}(\boldsymbol{n}',\phi')|\boldsymbol{r}\rangle = |\Re_{\boldsymbol{n}}(\phi)\Re_{\boldsymbol{n}'}(\phi')\boldsymbol{r}\rangle$$

Similarly

$$\hat{R}(\boldsymbol{n}',\phi')\hat{R}(\boldsymbol{n},\phi)|\boldsymbol{r}\rangle = |\Re_{\boldsymbol{n}'}(\phi')\Re_{\boldsymbol{n}}(\phi)\boldsymbol{r}\rangle$$

In general

$$\Re_{n}(\phi)\Re_{n'}(\phi') \neq \Re_{n'}(\phi')\Re_{n}(\phi) \text{ (geometrically),}$$

then

$$\underline{\hat{R}(\boldsymbol{n},\phi)\hat{R}(\boldsymbol{n}',\phi')|\boldsymbol{r}\rangle \neq \hat{R}(\boldsymbol{n}',\phi')\hat{R}(\boldsymbol{n},\phi)}$$

(c)

$$\hat{T}_d\hat{\pi}|\boldsymbol{r}\rangle = \hat{T}_d|-\boldsymbol{r}\rangle = |-\boldsymbol{r}+\boldsymbol{d}\rangle$$

$$\hat{\pi}\hat{T}_d|\boldsymbol{r}\rangle = \hat{\pi}|\boldsymbol{r}+\boldsymbol{d}\rangle = |-\boldsymbol{r}-\boldsymbol{d}\rangle$$

Therefore

$$\underline{\hat{T}_d\hat{\pi} \neq \hat{\pi}\hat{T}_d}$$

(d)

Since $[\hat{\pi},\hat{\boldsymbol{J}}]=0$

$$\hat{R}(\boldsymbol{n},\phi) = \exp\left(-\frac{i}{\hbar}\hat{\boldsymbol{J}}\cdot\boldsymbol{n}\phi\right)$$

$$\begin{aligned}\hat{\pi}\hat{R}(\boldsymbol{n},\phi)\hat{\pi} &= \hat{\pi}\exp\left(-\frac{i}{\hbar}\hat{\boldsymbol{J}}\cdot\boldsymbol{n}\phi\right)\hat{\pi} \\ &= \exp\left(-\frac{i}{\hbar}\hat{\pi}\hat{\boldsymbol{J}}\hat{\pi}\cdot\boldsymbol{n}\phi\right) \\ &= \exp\left(-\frac{i}{\hbar}\hat{\boldsymbol{J}}\cdot\boldsymbol{n}\phi\right) \\ &= \hat{R}(\boldsymbol{n},\phi)\end{aligned}$$

Then $\hat{R}(\boldsymbol{n},\phi)$ is commutable with $\hat{\pi}$.

((**Another method**))

$$\hat{R}\hat{\pi}|\mathbf{r}\rangle = \hat{R}|-\mathbf{r}\rangle = |-\Re\mathbf{r}\rangle$$

$$\hat{\pi}\hat{R}|\mathbf{r}\rangle = \hat{\pi}|\Re\mathbf{r}\rangle = |-\Re\mathbf{r}\rangle$$

$$\hat{R}\hat{\pi} = \hat{\pi}\hat{R}.$$

((4-3))

4.3 A quantum-mechanical state Ψ is known to be a simultaneous eigenstate of two Hermitian operators A and B that *anticommute*:

$$AB + BA = 0.$$

What can you say about the eigenvalues of A and B for state Ψ? Illustrate your point using the parity operator (which can be chosen to satisfy $\pi = \pi^{-1} = \pi^{\dagger}$) and the momentum operator.

((**Solution**))

$$\hat{A}|\Phi\rangle = \alpha|\Phi\rangle$$

$$\hat{B}|\Phi\rangle = \beta|\Phi\rangle$$

From anticommutation relation

$$(\hat{A}\hat{B} + \hat{B}\hat{A})|\Phi\rangle = (\alpha\beta + \beta\alpha)|\Phi\rangle = 2\alpha\beta|\Phi\rangle = 0 .$$

Then $\alpha = 0$ or $\beta = 0$.

We have the relation between $\hat{\pi}$ and $\hat{\boldsymbol{p}}$.

$$\hat{\pi}\hat{\boldsymbol{p}} + \hat{\boldsymbol{p}}\hat{\pi} = 0$$

$$\hat{\boldsymbol{p}}|\boldsymbol{p}'\rangle = \boldsymbol{p}'|\boldsymbol{p}'\rangle$$

$$(\hat{\pi}\hat{\boldsymbol{p}} + \hat{\boldsymbol{p}}\hat{\pi})|\boldsymbol{p}'\rangle = \hat{\pi}\boldsymbol{p}'|\boldsymbol{p}'\rangle + \hat{\boldsymbol{p}}\hat{\pi}|\boldsymbol{p}'\rangle$$

$$\hat{\boldsymbol{p}}(\hat{\pi}|\boldsymbol{p}'\rangle) = -\boldsymbol{p}'(\hat{\pi}|\boldsymbol{p}'\rangle)$$

Therefore $\hat{\pi}|\boldsymbol{p}'\rangle$ is the eigenket of $\hat{\boldsymbol{p}}$ with eigenvalue $-\boldsymbol{p}'$. Only the state $|\boldsymbol{p}'\rangle$ with $\boldsymbol{p}' = 0$ is a simultaneous eigenfunction of the parity operator $\hat{\pi}$ and the momentum $\hat{\boldsymbol{p}}$.

((4-4))

4.4 A spin $\frac{1}{2}$ particle is bound to a fixed center by a spherically symmetrical potential.

(a) Write down the spin-angular function $\mathcal{Y}_{l=0}^{j=1/2,m=1/2}$.

(b) Express $(\boldsymbol{\sigma}\cdot\mathbf{x})\,\mathcal{Y}_{l=0}^{j=1/2,m=1/2}$ in terms of some other $\mathcal{Y}_{l}^{j,m}$.

(c) Show that your result in (b) is understandable in view of the transformation properties of the operator $\mathbf{S}\cdot\mathbf{x}$ under rotations and under space inversion (parity).

((**Solution**))

The spin angular function in two component form is defined as follows.

$$y_l^{j=l+1/2,m}=\sqrt{\frac{l+m+1/2}{2l+1}}Y_l^{m-1/2}(\theta,\phi)\chi_+ +\sqrt{\frac{l-m+1/2}{2l+1}}Y_l^{m+1/2}(\theta,\phi)\chi_-$$

$$y_l^{j=l-1/2,m}=-\sqrt{\frac{l-m+1/2}{2l+1}}Y_l^{m-1/2}(\theta,\phi)\chi_+ +\sqrt{\frac{l+m+1/2}{2l+1}}Y_l^{m+1/2}(\theta,\phi)\chi_-$$

where $\chi_\pm$ is a two-component spinor (spinor wave function)

$$|+\rangle=\begin{pmatrix}1\\0\end{pmatrix}=\chi_+,\qquad |-\rangle=\begin{pmatrix}0\\1\end{pmatrix}=\chi_-$$

$$y_{l=0}^{j=1/2,m=1/2}=Y_0^0(\theta,\phi)\chi_+=\begin{pmatrix}Y_0^0(\theta,\phi)\\0\end{pmatrix}$$

where

$$Y_0^0(\theta,\phi)=\frac{1}{2\sqrt{\pi}}$$

$$(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{r}})Y_{l=0}^{j=1/2,m=1/2}=\begin{pmatrix}z & x-iy\\ x+iy & z\end{pmatrix}\begin{pmatrix}Y_0^0(\theta,\phi)\\0\end{pmatrix}=\begin{pmatrix}zY_0^0(\theta,\phi)\\(x+iy)Y_0^0(\theta,\phi)\end{pmatrix}$$

Here we note that

$$zY_0^0(\theta,\phi)=r\cos\theta\frac{1}{2\sqrt{\pi}}=r\frac{1}{\sqrt{3}}Y_1^0(\theta,\phi)$$

$$(x+iy)Y_0^0(\theta,\phi) = re^{i\phi}\sin\theta\frac{1}{2\sqrt{\pi}} = -\frac{1}{\sqrt{6}}rY_1^1(\theta,\phi)$$

Then we have

$$(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{r}})Y_{l=0}^{j=1/2,m=1/2} = \frac{r}{\sqrt{3}}\begin{pmatrix} Y_1^0(\theta,\phi) \\ -\sqrt{2}Y_1^1(\theta,\phi)\end{pmatrix} = -rY_{l=1}^{j=1/2,m=1/2}$$

where

$$Y_{l=1}^{j=1/2,m} = -\frac{1}{\sqrt{3}}Y_1^0(\theta,\phi)\chi_+ + \sqrt{\frac{2}{3}}Y_1^1(\theta,\phi)\chi_- = -\frac{1}{\sqrt{3}}\begin{pmatrix} Y_1^0(\theta,\phi) \\ -\sqrt{2}Y_1^1(\theta,\phi)\end{pmatrix}$$

when $m = 1/2$

$$\begin{aligned}
Y_{l=1}^{j=1/2,m=1/2} &= -\sqrt{\frac{1}{3}}Y_1^0(\theta,\phi)\chi_+ + \sqrt{\frac{2}{3}}Y_1^1(\theta,\phi)\chi_- \\
&= \begin{pmatrix} -\sqrt{\frac{1}{3}}Y_1^0(\theta,\phi) \\ \sqrt{\frac{2}{3}}Y_1^1(\theta,\phi)\end{pmatrix} \\
&= \frac{1}{\sqrt{3}}\begin{pmatrix} -Y_1^0(\theta,\phi) \\ \sqrt{2}Y_1^1(\theta,\phi)\end{pmatrix}
\end{aligned}$$

((**Note**))

$$Y_1^1(\theta,\phi) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{i\phi}, \quad Y_1^0(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta,$$

$$Y_1^{-1}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{-i\phi}$$

(b)

Parity operator:

Since $\hat{\pi}^+\hat{x}\hat{\pi} = -\hat{x}$, $\hat{\pi}^+\hat{\sigma}_x\hat{\pi} = \hat{\sigma}_x$

$$\hat{\pi}^+(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{r}})\hat{\pi} = -\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{r}}$$

$$|\psi'\rangle = (\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{r}})|\psi\rangle$$

$$\hat{\pi}|\psi'\rangle = \hat{\pi}(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{r}})\hat{\pi}^{-1}\hat{\pi}|\psi\rangle = -(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{r}})\hat{\pi}|\psi\rangle = -\lambda(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{r}})|\psi\rangle = -\lambda|\psi'\rangle$$

where $\hat{\pi}|\psi\rangle = \lambda|\psi\rangle$. Thus the parity of $|\psi'\rangle$ is different from that of $|\psi\rangle$.In fact,

$$\hat{\pi}|l,m\rangle = (-1)^l|l,m\rangle .$$

When l = 1. the wave function has the odd parity. When l = 0, the wave function has the even parity.

Rotation operator

Since $\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{r}}$ is a pseudo scalar operator, it is invariant under the rotation. From the Wigner –Eckart theorem,

$$\langle \alpha'; j', m'|\hat{T}_{q=0}^{(k=0)}|\alpha; j, m\rangle = \langle j, k=0; m, q=0| j, k=0; j', m'\rangle = 0$$

unless

$$m' = m \text{ and } j' = j$$

In fact, the value of m and j does not change before and after the operation $\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{r}}$.

((**Mathematica**))

```
Clear["Global`*"];
rule1 = {x → r Cos[φ] Sin[θ],
   y → r Sin[θ] Sin[φ], z → r Cos[θ]};
```

```
SphericalHarmonicY[0, 0, θ, ϕ]
```

$$\frac{1}{2\sqrt{\pi}}$$

```
z SphericalHarmonicY[0, 0, θ, ϕ] /.
   rule1 // Simplify
```

$$\frac{r\,\mathrm{Cos}[\theta]}{2\sqrt{\pi}}$$

```
(x + ⅈ y) SphericalHarmonicY[0, 0,
     θ, ϕ] /. rule1 // FullSimplify
```

$$\frac{e^{i\varphi}\, r\,\mathrm{Sin}[\theta]}{2\sqrt{\pi}}$$

```
Table[
 {m, SphericalHarmonicY[1, m, θ, ϕ]},
 {m, 1, -1, -1}]
```

$$\left\{\left\{1, -\frac{1}{2} e^{i \phi} \sqrt{\frac{3}{2 \pi}} \operatorname{Sin}[\theta]\right\},\right.$$

$$\left\{0, \frac{1}{2} \sqrt{\frac{3}{\pi}} \operatorname{Cos}[\theta]\right\},$$

$$\left.\left\{-1, \frac{1}{2} e^{-i \phi} \sqrt{\frac{3}{2 \pi}} \operatorname{Sin}[\theta]\right\}\right\}$$

((**4-5**))

4.5 Because of weak (neutral-current) interactions, there is a parity-violating potential between the atomic electron and the nucleus as follows:

$$V = \lambda[\delta^{(3)}(\mathbf{x})\mathbf{S}\cdot\mathbf{p} + \mathbf{S}\cdot\mathbf{p}\delta^{(3)}(\mathbf{x})],$$

where **S** and **p** are the spin and momentum operators of the electron, and the nucleus is assumed to be situated at the origin. As a result, the ground state of an alkali atom, usually characterized by $|n,l,j,m\rangle$, actually contains very tiny contributions from other eigenstates as follows:

$$|n,l,j,m\rangle \to |n,l,j,m\rangle + \sum_{n'l'j'm'} C_{n'l'j'm'}|n',l',j',m'\rangle.$$

On the basis of symmetry considerations *alone*, what can you say about (n',l',j',m'), which give rise to nonvanishing contributions? Suppose the radial wave functions and the energy levels are all known. Indicate how you may calculate $C_{n'l'j'm'}$. Do we get further restrictions on (n',l',j',m')?

((**Solution**))
From the perturbation theory,

$$C_{n',l',j'm'} = \frac{\langle n',l',j',m'|\hat{V}|n,l,j,m\rangle}{E_{n.l,j,m} - E_{n'.l',j',m}'}$$

Parity operator:
Since

$$\hat{\pi}^{+}\hat{p}_x\hat{\pi} = -\hat{p}_x, \qquad \hat{\pi}^{+}\hat{\sigma}_x\hat{\pi} = \hat{\sigma}_x$$

we have

$$\hat{\pi}^{+}(\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{p}})\hat{\pi} = -\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{p}},$$

$$|\psi'\rangle = (\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{p}})|\psi\rangle,$$

$$\hat{\pi}|\psi'\rangle = \hat{\pi}(\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{p}})\hat{\pi}^{-1}\hat{\pi}|\psi\rangle = -(\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{p}})\hat{\pi}|\psi\rangle = -\lambda(\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{p}})|\psi\rangle = -\lambda|\psi'\rangle$$

Thus the parity of $|\psi'\rangle$ is different from that of $|\psi\rangle$.

In fact, $\hat{\pi}\left|n,l,j,m\right\rangle = (-1)^l \left|n,l,j,m\right\rangle$. The transition between $\left|n.l.j,m\right\rangle$ and $\left|n.l'.j,m\right\rangle$ occurs only when l' - l = odd number.

Rotation operator

Since $\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{p}}$ is a pseudo scalar operator, it is invariant under the rotation. From the Wigner –Eckart theorem,

$$\left\langle n',l' j',m'\right|\hat{T}_{q=0}^{(k=0)}\left|n.l,j,m\right\rangle = \left\langle j,k=0;m,q=0\right|\left.j,k=0;j',m'\right\rangle = 0$$

unless

$$m' = m \text{ and } j' = j$$

In fact, the value of *m* and *j* does not change before and after the operation $\hat{\mathbf{S}}\cdot\hat{\mathbf{p}}$.

Since the perturbation potential is described by a Dirac Delta function, it is necessary for that transition that $R_{nl}(r=0)\neq 0$ and $R_{n'l}'(r=0)\neq 0$; l = 1 and l' = 0 or l = 0 and l' = 1.

In conclusion:

We have nonzero-matrix elements only for

$$\left\langle l'=0, j'=1/2, m'=\pm 1/2\right|\hat{V}\left|l=1, j=1/2, m=\pm 1/2\right\rangle \neq 0$$

and

$$\left\langle l=0, j=1/2, m=\pm 1/2\right|\hat{V}\left|l'=1, j'=1/2, m'=\pm 1/2\right\rangle \neq 0$$

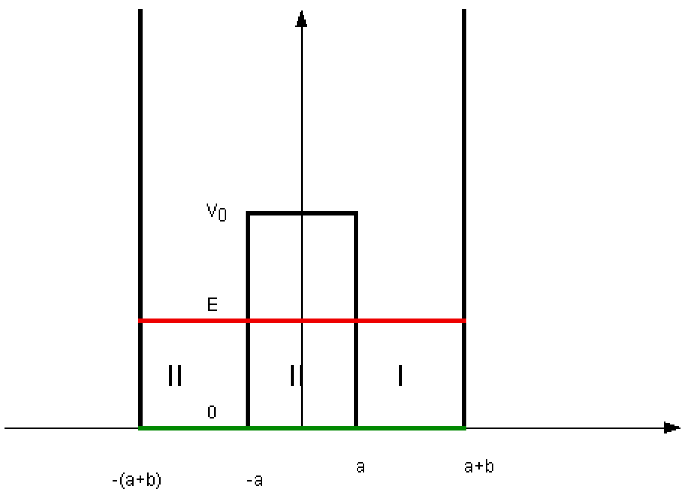
((4-6))

4.6 Consider a symmetric rectangular double-well potential:

$$V = \begin{cases} \infty & \text{for } |x| > a+b; \\ 0 & \text{for } a < |x| < a+b; \\ V_0 > 0 & \text{for } |x| < a. \end{cases}$$

Assuming that V_0 is very high compared to the quantized energies of low-lying states, obtain an approximate expression for the energy splitting between the two lowest-lying states.

((**Solution**))



When potential is an even function, the wave function should have even parity or odd parity.

$$[\hat{\pi}, \hat{H}] = 0$$

$\hat{\pi}$ is the parity operator.

$$\hat{\pi}^2 = 1 \qquad \hat{\pi}^+ = \hat{\pi} = \hat{\pi}^{-1}$$

$$\hat{\pi}\hat{x}\hat{\pi} = -\hat{x}\,. \qquad \hat{\pi}\hat{p}\hat{\pi} = -\hat{p}$$

$\hat{H}$ is the Hamiltonian.

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

$$\hat{\pi}\hat{H}\hat{\pi} = \hat{\pi}[\frac{\hat{p}^2}{2m} + V(\hat{x})]\hat{\pi}$$
$$= \frac{1}{2m}(\hat{\pi}\hat{p}\hat{\pi})^2 + V(\hat{\pi}\hat{x}\hat{\pi})$$
$$= \frac{1}{2m}(-\hat{p})^2 + V(-\hat{x})$$
$$= \frac{1}{2m}\hat{p}^2 + V(\hat{x})$$

since $V(-\hat{x}) = V(\hat{x})$

Then we have a simultaneous eigenket:

$$\hat{H}|\psi\rangle = E|\psi\rangle, \qquad \text{and} \qquad \hat{\pi}|\psi\rangle = \lambda|\psi\rangle$$

Since $\hat{\pi}^2 = 1$,

$$\hat{\pi}^2|\psi\rangle = \lambda\hat{\pi}|\psi\rangle = \lambda^2|\psi\rangle = |\psi\rangle$$

Thus we have $\lambda = \pm 1$.

or

$$\hat{\pi}|\psi\rangle = \pm|\psi\rangle$$

$$\langle x|\hat{\pi}|\psi\rangle = \pm\langle x|\psi\rangle$$

Since $\hat{\pi}|x\rangle = |-x\rangle$, or $\langle x|\hat{\pi}^+ = \langle x|\hat{\pi} = \langle -x|$

$$\langle -x|\psi\rangle = \pm\langle x|\psi\rangle$$

or

$$\psi(-x) = \pm\psi(x)$$

We need to solve the Schrödinger equation.

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

$$k^2 = \frac{2m}{\hbar^2} E , \qquad \rho^2 = \frac{2m}{\hbar^2}(V_0 - E)$$

or

$$(kb)^2 = \frac{2m}{\hbar^2} Eb^2 = \varepsilon , \qquad (\rho b)^2 = \frac{2m}{\hbar^2}(V_0 b^2 - Eb^2) = \nu_0{}^2 - \varepsilon$$

and

$$\nu_0{}^2 = \frac{2m}{\hbar^2}(V_0 b^2)$$

or

$$(kb)^2 + (\rho b)^2 = \nu_0{}^2 ,$$

(a) The wave function with even parity

$$\psi_I(x) = A\sin[k(x - a - b)]$$

$$\psi_{II}(x) = B\cosh(\rho x)$$

$$\psi_{III}(x) = -A\sin[k(x + a + b)]$$

$$\frac{d\psi_I(x)}{dx} = Ak\cos[k(x - a - b)]$$

$$\frac{d\psi_{II}(x)}{dx} = B\rho\sinh(\rho x)$$

((**Boundary condition**))

At $x = a$, $\psi(x)$ and $\frac{d\psi(x)}{dx}$ are continuous.

$$-A\sin(kb) - B\cosh(\rho a) = 0$$

$$Ak\cos(kb) = B\rho\sinh(a\rho)$$

We define the matrix *M*;

MX=0

where

$$M = \begin{pmatrix} -\sin(kb) & -\cosh(\rho a) \\ k\cos(kb) & -\rho\sinh(\rho a) \end{pmatrix}, \qquad X = \begin{pmatrix} A \\ B \end{pmatrix}$$

det$M$=0, leads to

$$k\cos(kb)\cosh(\rho a) + \rho\sin(kb)\sinh(\rho a) = 0$$

or

$$kb\coth(\rho b\frac{a}{b}) + \rho b\tan(kb) = 0$$

for the even parity

In summary

$$(kb)^2 + (\rho b)^2 = \nu_0{}^2,$$

$$kb\coth(\rho b\frac{a}{b}) + \rho b\tan(kb) = 0$$

For simplicity we use
$X = kb$, $Y = \rho b$,

(I)

$$X^2 + Y^2 = \nu_0{}^2, \tag{1}$$

$$X\coth(Y\frac{a}{b}) + Y\tan(X) = 0. \tag{2}$$

(b) The wave function with odd parity

$$\psi_I(x) = A\sin[k(x-a-b)]$$

$$\psi_{II}(x) = B\sinh(\rho x)$$

$$\psi_{III}(x) = -A\sin[k(x+a+b)]$$

$$\frac{d\psi_I(x)}{dx} = Ak\cos[k(x-a-b)]$$

$$\frac{d\psi_{II}(x)}{dx} = B\rho\cosh(\rho x)$$

$$\frac{d\psi_{III}(x)}{dx} = -Ak\cos[k(x+a+b)]$$

((Boundary condition))

At $x = a$, $\psi(x)$ and $\frac{d\psi(x)}{dx}$ are continuous.

$$-A\sin(kb) - B\sinh(\rho a) = 0$$

$$Ak\cos(bk) - B\rho\cosh(a\rho) = 0$$

We define the matrix M;

$$MX=0$$

where

$$M = \begin{pmatrix} -\sin(kb) & -\sinh(\rho a) \\ k\cos(kb) & -\rho\cosh(\rho a) \end{pmatrix}, \qquad X = \begin{pmatrix} A \\ B \end{pmatrix}$$

det$M$=0 leads to

$$k\cos(kb)\sinh(\rho a) + \rho\sin(kb)\cosh(\rho a) = 0$$

or

$$kb\tanh(\rho b\frac{a}{b}) + \rho b\tan(kb) = 0$$

for the odd parity

In summary

$$(kb)^2 + (\rho b)^2 = \nu_0{}^2,$$
$$kb\tanh(\rho b\frac{a}{b}) + \rho b\tan(kb) = 0$$

For simplicity we use

$$X = ka,\ Y = \rho a,$$

(II)

$$X^2 + Y^2 = \nu_0{}^2,$$

$$X \tanh(Y \frac{a}{b}) + Y \tan(X) = 0\,. \qquad (3)$$

Case-1

In the limit of $\nu_0 \to \infty$ ($V_0 = \infty$), $X = n\pi$ for both the symmetric and antisymmetric wave functions. Therefore the energy level is degenerate.

$$X^2 = (kb)^2 = \frac{2m}{\hbar^2} Eb^2 = \varepsilon = (n\pi)^2, \quad \text{or} \quad E = \frac{\hbar^2}{2m}\left(\frac{n\pi}{b}\right)^2 \text{ with } n = \pm 1, \pm 2, \pm 3,$$

Case-2

In the limit of ν_0, the value of X for the symmetrical wave function is a little lower than that for the antisymmetrical wave function. The solution of $X = 0$ is not included because the wavefunction becomes zero.

$$\frac{b}{a} = 2\,.$$

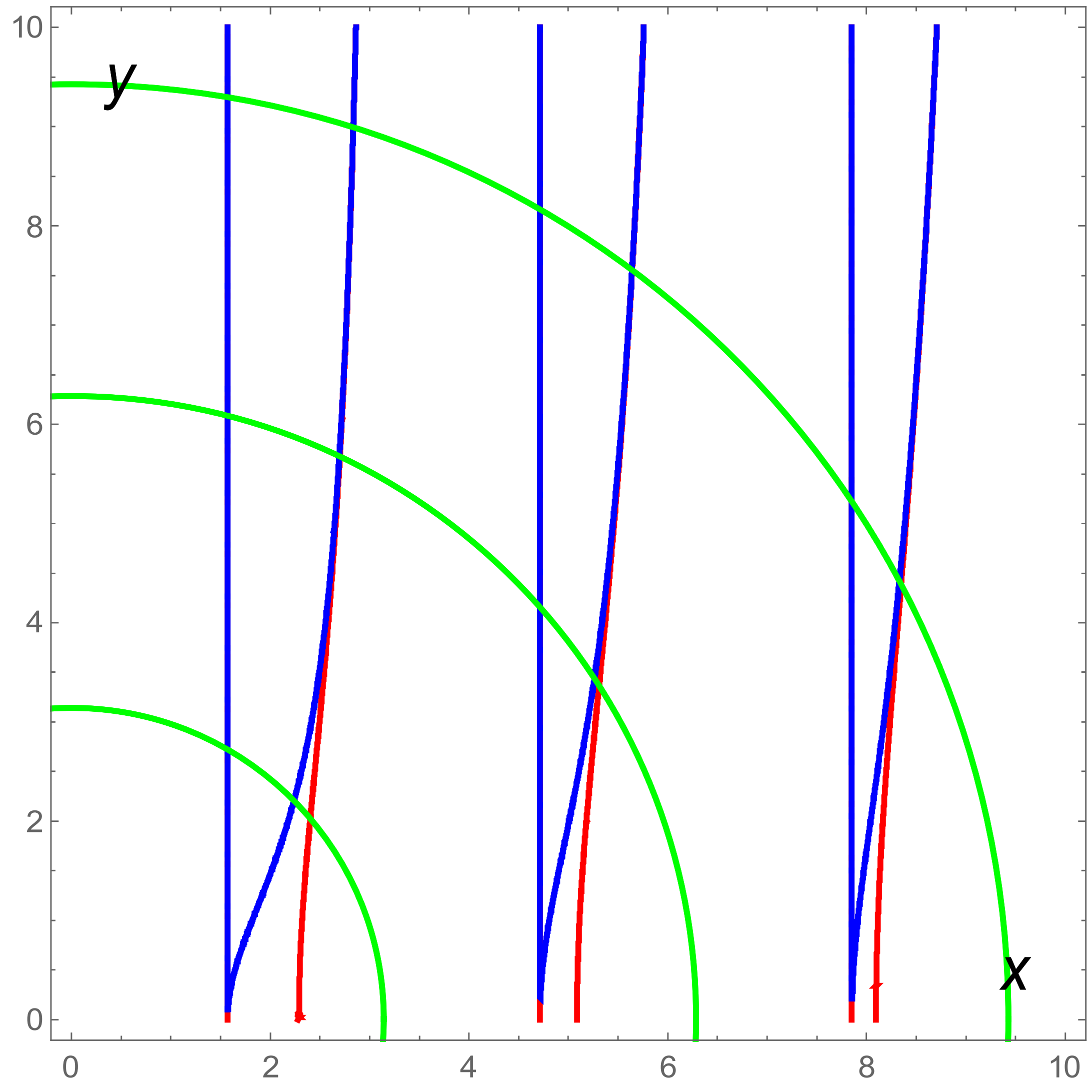


Fig. Solutions with the even parity (red) and with the odd parity (green). The green circle with $x^2 + y^2 = \nu_0{}^2$

((4-7))

4.7 (a) Let $\psi(\mathbf{x},t)$ be the wave function of a spinless particle corresponding to a plane wave in three dimensions. Show that $\psi^*(\mathbf{x},-t)$ is the wave function for the plane wave with the momentum direction reversed.

(b) Let $\chi(\hat{\mathbf{n}})$ be the two-component eigenspinor of $\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}$ with eigenvalue $+1$. *Using the explicit form of* $\chi(\hat{\mathbf{n}})$ (in terms of the polar and azimuthal angles β and γ that characterize $\hat{\mathbf{n}}$), verify that $-i\sigma_2\chi^*(\hat{\mathbf{n}})$ is the two-component eigenspinor with the spin direction reversed.

((**Solution**))

(a)

$$\phi_{\mathbf{p}}(\mathbf{r},t) = \frac{1}{(2\pi\hbar)^{3/2}}\exp\left(\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r} - i\frac{E}{\hbar}t\right)$$

$$\phi_{\boldsymbol{p}}^*(\boldsymbol{r},-t) = \frac{1}{(2\pi\hbar)^{3/2}}\exp\left(-\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r} - i\frac{E}{\hbar}t\right)$$

$$\phi_{-\boldsymbol{p}}(\boldsymbol{r},t) = \frac{1}{(2\pi\hbar)^{3/2}}\exp\left(-\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r} - i\frac{E}{\hbar}t\right)$$

$$\phi_{\boldsymbol{p}}^*(\boldsymbol{r},-t) = \phi_{-\boldsymbol{p}}(\boldsymbol{r},t)$$

(b)

$$|+\rangle_n = \begin{pmatrix} e^{-i\alpha/2}\cos\frac{\beta}{2} \\ e^{i\alpha/2}\sin\frac{\beta}{2} \end{pmatrix}, \quad |-\rangle_n = \begin{pmatrix} e^{-i\alpha/2}\sin\frac{\beta}{2} \\ e^{i\alpha/2}\cos\frac{\beta}{2} \end{pmatrix}$$

$$\hat{\Theta} = -i\hat{\sigma}_y\hat{K}$$

$$\hat{\Theta}|+\rangle_n = -i\hat{\sigma}_y\hat{K}[e^{-i\alpha/2}\cos\frac{\beta}{2}|+\rangle + e^{i\alpha/2}\sin\frac{\beta}{2}|-\rangle]$$
$$= -i\hat{\sigma}_y[^{i\alpha/2}\cos\frac{\beta}{2}|+\rangle + e^{-i\alpha/2}in\frac{\beta}{2}|-\rangle]$$

Since $\hat{\sigma}_y|+\rangle = i|-\rangle$, $\hat{\sigma}_y|-\rangle = -i|+\rangle$,

$$\hat{\Theta}|+\rangle_n = e^{i\alpha/2}\cos\frac{\beta}{2}|-\rangle - e^{-i\alpha/2}\sin\frac{\beta}{2}|+\rangle = |-\rangle_n$$

((**4-8**))

4.8 (a) Assuming that the Hamiltonian is invariant under time reversal, prove that the wave function for a spinless nondegenerate system at any given instant of time can always be chosen to be real.

(b) The wave function for a plane-wave state at $t = 0$ is given by a complex function $e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}$. Why does this not violate time-reversal invariance?

((**Solution**))

(a)

$$\hat{H}\hat{\Theta} = \hat{\Theta}\hat{H}$$

$$\hat{H}\hat{\Theta}|\boldsymbol{n}\rangle = \hat{\Theta}\hat{H}|\boldsymbol{n}\rangle = E_n\hat{\Theta}|\boldsymbol{n}\rangle$$

$\hat{\Theta}|\boldsymbol{n}\rangle$ is the eigenket of $\hat{H}$ with E_n.
Since $|\boldsymbol{n}\rangle$ is not degenerate

$$|\widetilde{\boldsymbol{n}}\rangle = \hat{\Theta}|\boldsymbol{n}\rangle = |\boldsymbol{n}\rangle$$

$$\langle\widetilde{\boldsymbol{r}}|\widetilde{\boldsymbol{n}}\rangle = \langle\boldsymbol{n}|\boldsymbol{r}\rangle .$$

Since

$$|\widetilde{\boldsymbol{r}}\rangle = \Theta|\boldsymbol{r}\rangle = |\boldsymbol{r}\rangle,$$

we have

$$\langle\boldsymbol{r}|\boldsymbol{n}\rangle = \langle\boldsymbol{n}|\boldsymbol{r}\rangle = \langle\boldsymbol{r}|\boldsymbol{n}\rangle^*$$

=> $\langle\boldsymbol{r}|\boldsymbol{n}\rangle$ is real.

(b)

$$|\boldsymbol{n}\rangle = |\boldsymbol{p}'\rangle$$

$$\hat{H}|\boldsymbol{n}\rangle = \hat{H}|\boldsymbol{p}'\rangle = \frac{p^2}{2}|\boldsymbol{p}'\rangle$$

$E_{p'} = E_{-p'}$ => $|\boldsymbol{p}'\rangle$ and $|-\boldsymbol{p}'\rangle$ are the eigenket of $\hat{H}$ with the same energy. But $|\boldsymbol{p}'\rangle$ and $|-\boldsymbol{p}'\rangle$ are different states.

$$\langle -\boldsymbol{p}'|\boldsymbol{p}'\rangle = 0$$

$$(\hat{\Theta}|\boldsymbol{p}'\rangle = |-\boldsymbol{p}'\rangle)$$

=> $\langle \boldsymbol{r}|\boldsymbol{p}'\rangle$ is not a real but a complex number.

((**4-9**))

4.9 Let $\phi(\mathbf{p}')$ be the momentum-space wave function for state $|\alpha\rangle$—that is, $\phi(\mathbf{p}') = \langle \mathbf{p}'|\alpha\rangle$. Is the momentum-space wave function for the time-reversed state $\theta|\alpha\rangle$ given by $\phi(\mathbf{p}')$, by $\phi(-\mathbf{p}')$, by $\phi^*(\mathbf{p}')$, or by $\phi^*(-\mathbf{p}')$? Justify your answer.

((**Solution**))

Since $\hat{\Theta}|-p'\rangle = |p'\rangle$

$$\langle \tilde{p}'|\tilde{\alpha}\rangle = \langle p'|\alpha\rangle^*$$

or

$$\langle -p'|\tilde{\alpha}\rangle = \langle p'|\alpha\rangle^*$$

or

$$\langle p'|\tilde{\alpha}\rangle = \langle -p'|\alpha\rangle^*$$

4.10

4.10 **(a)** What is the time-reversed state corresponding to $\mathcal{D}(R)|j,m\rangle$?

(b) Using the properties of time reversal and rotations, prove

$$\mathcal{D}^{(j)*}_{m'm}(R) = (-1)^{m-m'}\mathcal{D}^{(j)}_{-m',-m}(R).$$

(c) Prove $\theta|j,m\rangle = i^{2m}|j,-m\rangle$.

((**Solution**))

We use the following definition.

$$\langle j,m'|\hat{R}|j,m\rangle = D^{(j)}_{m',m}(\hat{R})$$

(a)

$$\hat{\Theta}\hat{\boldsymbol{J}}\hat{\Theta}^{-1} = -\hat{\boldsymbol{J}}$$

$$\hat{\Theta}\hat{J}_z\hat{\Theta}^{-1} = -\hat{J}_z, \qquad \hat{\Theta}\hat{J}_x\hat{\Theta}^{-1} = -\hat{J}_x, \qquad \hat{\Theta}\hat{J}_y\hat{\Theta}^{-1} = -\hat{J}_y$$

$$\hat{\Theta}\hat{J}_+\hat{\Theta}^{-1} = \hat{\Theta}(\hat{J}_x + i\hat{J}_y)\hat{\Theta}^{-1} = -(\hat{J}_x - i\hat{J}_y) = -\hat{J}_-$$

$$\hat{\Theta}\hat{J}_-\hat{\Theta}^{-1} = \hat{\Theta}(\hat{J}_x - i\hat{J}_y)\hat{\Theta}^{-1} = -(\hat{J}_x + i\hat{J}_y) = -\hat{J}_+$$

or

$$\hat{J}_z\hat{\Theta} = -\hat{\Theta}\hat{J}_z, \qquad \hat{J}_+\hat{\Theta} = -\hat{\Theta}\hat{J}_-, \qquad \hat{J}_-\hat{\Theta} = -\hat{\Theta}\hat{J}_+$$

Since

$$\hat{J}_z\hat{\Theta}|j,m\rangle = -\hat{\Theta}\hat{J}_z|j,m\rangle = \hbar(-m)\hat{\Theta}|j,m\rangle$$

$\hat{\Theta}|j,m\rangle$ is the eigenket of $\hat{J}_z$ with the eigenvalue (-*m*); $\hat{\Theta}|j,m\rangle \propto |j,-m\rangle$. We also have

$$\hat{J}_+\hat{\Theta}|j,m\rangle = -\hat{\Theta}\hat{J}_-|j,m\rangle = -\hbar\sqrt{(j+m)(j-m+1)}\hat{\Theta}|j,m-1\rangle$$

$$\hat{J}_-\hat{\Theta}|j,m\rangle = -\hat{\Theta}\hat{J}_+|j,m\rangle = -\hbar\sqrt{(j-m)(j+m+1)}\hat{\Theta}|j,m+1\rangle$$

Suppose that $,\hat{\Theta}|j,m\rangle = i^{2m}|j,-m\rangle$, then we have the

$$\hat{J}_+|j,-m\rangle = \hbar\sqrt{(j+m)(j-m+1)}|j,-m+1\rangle$$

$$\hat{J}_-|j,-m\rangle = \hbar\sqrt{(j-m)(j+m+1)}|j,-m-1\rangle$$

Note that $|\tilde{\alpha}\rangle = \hat{\Theta}|j,m\rangle = i^{2m}|j,-m\rangle$, $|\alpha\rangle = |j,m\rangle$, satisfying the normalization condition.

$$\langle\tilde{\alpha}|\tilde{\alpha}\rangle = \langle\alpha|\alpha\rangle = 1$$

(b)

$$\hat{R}(\boldsymbol{n},\phi) = \exp[-\frac{i\phi}{\hbar}(\hat{\boldsymbol{J}}\cdot\boldsymbol{n})]$$

$$\begin{aligned}\hat{\Theta}\hat{R}(\boldsymbol{n},\phi)\hat{\Theta}^{-1} &= \exp[-\frac{\phi}{\hbar}\hat{\Theta}(i\hat{\boldsymbol{J}}\hat{\Theta}^{-1})\cdot\boldsymbol{n}] \\ &= \exp[-\frac{\phi}{\hbar}(\hat{\Theta}i\hat{\Theta}^{-1})(\hat{\Theta}\hat{\boldsymbol{J}}\hat{\Theta}^{-1})\cdot\boldsymbol{n}] \\ &= \exp[-\frac{i\phi}{\hbar}\hat{\boldsymbol{J}}\cdot\boldsymbol{n}] \\ &= \hat{R}(\boldsymbol{n},\phi)\end{aligned}$$

or

since $\hat{\Theta}i\hat{\Theta}^{-1} = -i\hat{1}$, and $\hat{\Theta}\hat{\boldsymbol{J}}\hat{\Theta}^{-1} = -\hat{\boldsymbol{J}}$. Then we get

$$\hat{\Theta}\hat{R}(\boldsymbol{n},\phi) = \hat{R}(\boldsymbol{n},\phi)\hat{\Theta}$$

We note that

$$\hat{\Theta}\hat{R}|j,m\rangle = \hat{R}\hat{\Theta}|j,m\rangle = i^{2m}\hat{R}|j,-m\rangle$$

We calculate the matrix element

$$\begin{aligned}\langle j,-m'|\hat{R}\hat{\Theta}|j,m\rangle &= i^{2m}\langle j,-m'|\hat{R}|j,-m\rangle \\ &= i^{2m}D^{(j)}_{-m',-m}(\hat{R})\end{aligned}$$

and

$$\langle j,-m'|\hat{\Theta}\hat{R}|j,m\rangle = \langle j,-m'|\hat{\Theta}\sum_{m''}|j,m''\rangle\langle j,m''|\hat{R}|j,m\rangle$$

$$= \sum_{m''}\langle j,-m'|\hat{\Theta}|j,m''\rangle\langle j,m''|\hat{R}|j,m\rangle^*$$

$$= \sum_{m''} i^{2m''}\langle j,-m'|j,-m''\rangle\langle j,m''|\hat{R}|j,m\rangle^*$$

$$= \sum_{m''} i^{2m''}\delta_{m',m''}\langle j,m''|\hat{R}|j,m\rangle^*$$

$$= i^{2m'}\langle j,m'|\hat{R}|j,m\rangle^*$$

$$= i^{2m'} D^{(j)}_{m',m}{}^*(R)$$

From these two equations, we have

$$i^{2m} D^{(j)}_{-m',-m}(R) = i^{2m'} D^{(j)}_{m',m}{}^*(R)$$

or

$$D^{(j)}_{m',m}{}^*(R) = i^{2(m-m')} D^{(j)}_{-m',-m}(R) = (-1)^{m-m'} D^{(j)}_{-m',-m}(R)$$

(c)

$$\hat{\Theta}^2|j,m\rangle = \hat{\Theta} i^{2m}|j,-m\rangle$$

$$= (-i)^{2m}\hat{\Theta}|j,-m\rangle$$

$$= (-i)^{2m}(i)^{2m}|j,m\rangle$$

$$= (-1)^{2m}|j,m\rangle$$

4.11

4.11 Suppose a spinless particle is bound to a fixed center by a potential $V(\mathbf{x})$ so asymmetrical that no energy level is degenerate. Using time-reversal invariance, prove

$$\langle \mathbf{L} \rangle = 0$$

for any energy eigenstate. (This is known as **quenching** of orbital angular momentum.) If the wave function of such a nondegenerate eigenstate is expanded as

$$\sum_l \sum_m F_{lm}(r) Y_l^m(\theta, \phi),$$

what kind of phase restrictions do we obtain on $F_{lm}(r)$?

((**Solution**))

Since $\hat{H}$ is invariant under time reversal,

$$\hat{\Theta}\hat{H}\hat{\Theta}^{-1} = \hat{H}\,, \qquad \text{or} \qquad \hat{\Theta}\hat{H} = \hat{H}\hat{\Theta}$$

When $|\phi_n\rangle$ is an eigenstate of $\hat{H}$ with the energy eigenvalue E_n,

$$\hat{H}\hat{\Theta}|\phi_n\rangle = \hat{\Theta}\hat{H}|\phi_n\rangle = E_n\hat{\Theta}|\phi_n\rangle$$

Thus $\hat{\Theta}|\phi_n\rangle$ is also the eigenstate of $\hat{H}$ with the energy eigenvalue E_n. Suppose that $|\phi_n\rangle$ is the non-degenerate state. Then we have

$$|\tilde{\phi}_n\rangle = \hat{\Theta}|\phi_n\rangle$$

The average of the orbital angular momentum is evaluated using the formula,

$$\langle \phi_n|\hat{\boldsymbol{L}}|\phi_n\rangle = \langle \tilde{\phi}_n|\hat{\Theta}\hat{\boldsymbol{L}}\hat{\Theta}^{-1}|\tilde{\phi}_n\rangle = -\langle \tilde{\phi}_n|\hat{\boldsymbol{L}}|\tilde{\phi}_n\rangle = -\langle \phi_n|\hat{\boldsymbol{L}}|\phi_n\rangle$$

since

$$\hat{\Theta}\hat{\boldsymbol{L}}\hat{\Theta}^{-1} = -\hat{\boldsymbol{L}}\,.$$

Then we have

$$\langle \phi_n|\hat{\boldsymbol{L}}|\phi_n\rangle = 0 \qquad \text{(quenching of the orbital angular momentum).}$$

Suppose that the wavefunction of the non-degenerate state is given by

$$\langle \boldsymbol{r} | \phi_n \rangle = \sum_{l,m} F_{lm}(r) Y_l^m(\theta, \phi) \tag{1}$$

and

$$\langle \boldsymbol{r} | \hat{\Theta} | \phi_n \rangle = \langle \tilde{\boldsymbol{r}} | \tilde{\phi}_n \rangle = \langle \boldsymbol{r} | \phi_n \rangle^* = \sum_{l,m} F_{lm}^*(r) [Y_l^m(\theta, \phi)]^* = \sum_{l,m} F_{lm}^*(r)(-1)^m Y_l^{-m}(\theta, \phi) \tag{2}$$

where $\hat{\Theta} |\boldsymbol{r}\rangle = |\tilde{\boldsymbol{r}}\rangle = |\boldsymbol{r}\rangle$. In the present case, Eqs.(1) and (2) are equal except for the phase factor;

since

$$\sum_{l,m} F_{lm}^*(r)(-1)^m Y_l^{-m}(\theta, \phi) = \sum_{l,m} F_{l,-m}^*(r)(-1)^m Y_l^m(\theta, \phi)$$

Thus we have

$$F_{lm}(r) = e^{i\alpha}(-1)^m F_{l,-m}^*(r)$$

4.12

4.12 The Hamiltonian for a spin 1 system is given by

$$H = AS_z^2 + B(S_x^2 - S_y^2).$$

Solve this problem *exactly* to find the normalized energy eigenstates and eigenvalues. (A spin-dependent Hamiltonian of this kind actually appears in crystal physics.) Is this Hamiltonian invariant under time reversal? How do the normalized eigenstates you obtained transform under time reversal?

((Solution))

We note that $[\hat{H}, \hat{\Theta}] = 0$

The Hamiltonian is given by

$$\hat{H} = \hbar^2 \begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix}$$

$$\hat{H}|1,1\rangle = \hbar^2 [A|1,1\rangle + B|1,-1\rangle] \qquad (1)$$

$\hat{H}|1,0\rangle = 0$ $\qquad$ ($|1,0\rangle$ is the eigenstate of $\hat{H}$ with the eigenvalue 0)

$$\hat{H}|1,-1\rangle = \hbar^2 [B|1,1\rangle + A|1,-1\rangle] \qquad (2)$$

In the subspace of $\{|1,1\rangle$ and $|1,-1\rangle\}$, the Hamiltonian can be written as

$$\begin{aligned}
\hat{H}_{sub} &= \hbar^2 \begin{pmatrix} A & B \\ B & A \end{pmatrix} \\
&= A\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + B\hbar^2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&= \hbar^2 (A\hat{1} + B\hat{\sigma}_x)
\end{aligned}$$

$$\hat{H}_{sub}|\pm x\rangle = \hbar^2 (A\hat{1} + B\hat{\sigma}_x)|\pm x\rangle = \hbar^2 (A \pm B)|\pm x\rangle$$

with

$$|+x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \qquad \text{(eigenvalue: } (A+B)\hbar^2\text{)}$$

$$|-x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \qquad \text{(eigenvalue: } (A-B)\hbar^2\text{)}$$

In summary we have three states

$$|\phi_1\rangle = |1,0\rangle \qquad \text{(energy eigenvalue, 0)}$$

$$|\phi_2\rangle = \frac{1}{\sqrt{2}}[|1,1\rangle + |1,-1\rangle] \qquad \text{(energy eigenvalue: } (A+B)\hbar^2\text{)}$$

$$|\phi_3\rangle = \frac{1}{\sqrt{2}}[|1,1\rangle - |1,-1\rangle] \qquad \text{(energy eigenvalue: } (A-B)\hbar^2\text{)}$$

The time reversal states:

$$\hat{\Theta}|\phi_1\rangle = \hat{\Theta}|1,0\rangle = |1,0\rangle$$

$$\hat{\Theta}|\phi_2\rangle = \frac{1}{\sqrt{2}}\hat{\Theta}[|1,1\rangle + |1,-1\rangle] = \frac{1}{\sqrt{2}}[(-1)|1,-1\rangle + (-1)^{-1}|1,1\rangle] = -|\phi_2\rangle$$

$$\hat{\Theta}|\phi_3\rangle = \frac{1}{\sqrt{2}}\hat{\Theta}[|1,1\rangle - |1,-1\rangle] = \frac{1}{\sqrt{2}}[(-1)|1,-1\rangle - (-1)^{-1}|1,1\rangle] = |\phi_3\rangle$$

((**Mathematica**))

```
Clear["Global`*"]; j = 1;
Jx[j_, n_, m_] := ℏ/2 Sqrt[(j - m) (j + m + 1)] KroneckerDelta[n, m + 1] +
   ℏ/2 Sqrt[(j + m) (j - m + 1)] KroneckerDelta[n, m - 1];
Jy[j_, n_, m_] := -ℏ/2 ⅈ Sqrt[(j - m) (j + m + 1)] KroneckerDelta[n, m + 1] +
   ℏ/2 ⅈ Sqrt[(j + m) (j - m + 1)] KroneckerDelta[n, m - 1];
Jz[j_, n_, m_] := ℏ m KroneckerDelta[n, m];
Jx = Table[Jx[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Jy = Table[Jy[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Jz = Table[Jz[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
```

```
Jx // MatrixForm
```

$$\begin{pmatrix} 0 & \frac{\hbar}{\sqrt{2}} & 0 \\ \frac{\hbar}{\sqrt{2}} & 0 & \frac{\hbar}{\sqrt{2}} \\ 0 & \frac{\hbar}{\sqrt{2}} & 0 \end{pmatrix}$$

```
Jy // MatrixForm
```

$$\begin{pmatrix} 0 & -\frac{i\hbar}{\sqrt{2}} & 0 \\ \frac{i\hbar}{\sqrt{2}} & 0 & -\frac{i\hbar}{\sqrt{2}} \\ 0 & \frac{i\hbar}{\sqrt{2}} & 0 \end{pmatrix}$$

```
Jz // MatrixForm
```

$$\begin{pmatrix} \hbar & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\hbar \end{pmatrix}$$

```
H1 = A1 Jz.Jz + B1 (Jx.Jx - Jy.Jy) // Simplify
```

$$\left\{\left\{A1\,\hbar^2,\ 0,\ B1\,\hbar^2\right\},\ \{0,\ 0,\ 0\},\ \left\{B1\,\hbar^2,\ 0,\ A1\,\hbar^2\right\}\right\}$$

```
H1 // MatrixForm
```

$$\begin{pmatrix} A1\,\hbar^2 & 0 & B1\,\hbar^2 \\ 0 & 0 & 0 \\ B1\,\hbar^2 & 0 & A1\,\hbar^2 \end{pmatrix}$$

```
Eigensystem[H1]
```

$$\left\{\left\{0,\ (A1 - B1)\,\hbar^2,\ (A1 + B1)\,\hbar^2\right\},\ \{\{0,\ 1,\ 0\},\ \{-1,\ 0,\ 1\},\ \{1,\ 0,\ 1\}\}\right\}$$