Homework Assignment #8

Math Methods

Due: Monday, Novermber 1st, midnight

Instructions:

Reading Quiz #6 is due by the start of class on Wednesday, November 10th. It covers the rest of chapter 4 (except normal modes).

Below is the a list of questions and problems from the texbook. It is not sufficient to simply obtain the correct answer. You must also explain your calculation, and each step so that it is clear that you understand the material.

Homework should be written legibly, on standard size paper. Do not write your homework up on scrap paper. If your work is illegible, it will be given a zero.

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1. Byron & Fuller, Chapter 4, problem 4.
2. Byron & Fuller, Chapter 4, problem 6.
3. Byron & Fuller, Chapter 4, problem 17.
4. Consider the three vectors

$$\begin{aligned} \vec{v}_1 &= \hat{\imath} + \hat{\jmath} + \hat{k} \\ \vec{v}_2 &= \hat{\imath} + 2\,\hat{\jmath} + 3\,\hat{k} \\ \vec{v}_3 &= \hat{\imath} + 2\,\hat{\jmath} + \hat{k} \end{aligned}$$

   Perform Gram-Schmidt orthonormalization on the set $\{\vec{v}_1, \vec{v}_2, \vec{v}_3\}$, starting with $\vec{v}_1$ as your first basis vector.

5. *Spinors:* Spin is often introduced in undergraduate physics courses simply as a 2-vector. This can be a bit confusing. Let's see why.

   In problem 28 from chapter 3 you learned that the operator $\hat{\mathcal{T}} \equiv e^{a\,\partial_x}$ is the *translation operator*, in that

$$\hat{\mathcal{T}}\, f(x) = f(x+a)$$

   In quantum mechanics this is written as:

$$\hat{\mathcal{T}} \equiv e^{ia\hat{p}_x/\hbar}$$

   since $\hat{p}_x = -i\hbar\partial_x$. This is stated as "the momentum operator is the *generator* of translations." In a similar fashion one can show that the generator of infinitesimal[1] rotations about the z axis is the operator $\hat{L}_z$, the operator which gives the z component of the angular momentum, so that to rotate something in quantum mechanics about the z-axis by an infinitesimal angle $\Delta\phi$ one can use the operator.

$$\hat{R}_z = e^{-i\hat{L}_z\Delta\phi/\hbar}$$

[1] We have to be a little careful since while translation operators are Abelian, rotation operators are not.

What about spin?

By analogy, the operator to rotate a spin about an arbitrary axis defined by the unit vector $\hat{n}$, is given by:

$$\hat{R}_{\hat{n}}(\Delta\phi) = \exp\left(\frac{-i\hat{\mathcal{S}}\cdot\hat{n}\,\Delta\phi,}{\hbar}\right) = \exp\left(\frac{-i\hat{\sigma}\cdot\hat{n}\,\Delta\phi}{2}\right)$$

where we have set the spin operator $\hat{\mathcal{S}} \to \hbar\hat{\sigma}/2$, the spin-1/2 operator made from the three Pauli matrices. Note that we have implicitly assumed our basis to the along the z-axis, with basis states:

$$|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix} \qquad\qquad |\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

(a) Show that

$$(\hat{\sigma}\cdot\hat{n})^k = \begin{cases} 1 & \text{k is even} \\ \hat{\sigma}\cdot\hat{n} & \text{k is odd} \end{cases}$$

(b) From the above prove that for the spin-1/2 case

$$\hat{R}_{\hat{n}}(\Delta\phi) = \cos\frac{\Delta\phi}{2} - i\,\sin\frac{\Delta\phi}{2}\hat{n}\cdot\hat{\sigma}$$

(c) If we repeatedly rotate about the same axis $\hat{n}$, then we know that rotations simply add, and we can write the general rotation matrix for an angle ϕ in the z-axis basis:

$$\begin{pmatrix} \cos\frac{\phi}{2} - i\,n_z\sin\frac{\phi}{2} & (-i\,n_x - n_y)\sin\frac{\phi}{2} \\ (-i\,n_x + n_y)\sin\frac{\phi}{2} & \cos\frac{\phi}{2} + i\,n_z\sin\frac{\phi}{2} \end{pmatrix}$$

(d) Using this matrix, what do you get if you rotate the state $|\uparrow\rangle$:

i. by $\pi/2$ about the x-axis?

ii. by π about the x-axis?

iii. by 2π about the x-axis?

(e) Does the state $|\uparrow\rangle$ rotate as a vector?

6. **Variational Calculations:** Consider the one dimensional Schrödinger equation, already converted to dimensionless units:

$$\mathcal{H}\psi(x) = \left\{-\frac{d^2}{dx^2} - \frac{1}{1+x^2}\right\}\psi(x) = E\,\psi(x)$$

with the boundary conditions $\psi(-\infty) = \psi(\infty) = 0$. We will assume a variational form for the groundstate:

$$\psi(x) = \sqrt{\frac{2\alpha^3}{\pi}}\frac{1}{x^2+\alpha^2}$$

where α is a constant that must be determined.

(a) Show that $\psi(x;\alpha)$ is normalized in the infinite interval.

(b) We wish to determine the value of α in a variational fashion so that:

$$\mathcal{I} \equiv \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

is a maximum. Evaluate an analytic expression for $\mathcal{I}(\alpha)$.

(c) Either plot your function and find its minimum, or take the dervivative and determine where it crosses zero. What is this value of α? Use this value of α to find an estimate of the smallest eigenvalue.

(d) Determine the groundstate eigenvalue directly by a numerical solution of the problem, using the eigenvalue solver for the Schrodinger equation that you developed in an earlier homework. Compare it to the value obtain from the variational calculation.

This problem is a bit tedious. You may question the wisdom of doing a variational calculation, since it required numerical evaluations only slightly simpler than writing an eigenvalue solver. On the other hand, eigenvalue solvers become much harder in two and three dimensions, whereas a good variational calculation is often much simpler.

4. Given $\mathbb{A} = e^{i\mathbb{B}}$

$$= \sum_{n=0}^{\infty} \frac{(i\mathbb{B})^n}{n!} = \mathbb{1} + i\mathbb{B} + \frac{(i\mathbb{B})^2}{2!} + \dots$$

and $\mathbb{B}$ is self-adjoint, then $\mathbb{A}$ is isometric & that any isometry U can be written as e^{iH} where H is Hermitian.

$$\mathbb{A}^\dagger = \sum_{n=0}^{\infty} \left[\frac{(i\mathbb{B})^n}{n!}\right]^\dagger = \sum_{n=0}^{\infty} \frac{(-i\mathbb{B}^\dagger)^n}{n!} = \sum_{n=0}^{\infty} \frac{(-i\mathbb{B})^n}{n!}$$

$$= e^{-i\mathbb{B}} = \left(e^{i\mathbb{B}}\right)^{-1}$$

If U is an isometry, then $\exists$ a similarity transformation $\mathbb{P}$ such that

$$\mathbb{P}^{-1} U \mathbb{P} = \begin{pmatrix} e^{i\theta_1} & & \tilde{0} \\ & e^{i\theta_2} & \\ & \ddots & \\ \tilde{0} & & e^{i\theta_n} \end{pmatrix} = e^{i\Theta}$$

where $\Theta = \begin{pmatrix} \theta_1 & & \tilde{0} \\ & \theta_2 & \\ \tilde{0} & \ddots & \theta_n \end{pmatrix}$

$$U = \mathbb{P} e^{i\Theta} \mathbb{P}^{-1} = \mathbb{P} \left\{ \mathbb{1} + i\Theta + \frac{(i\Theta)(i\Theta)}{2!} + \dots \right\} \mathbb{P}^{-1}$$

$$= \mathbb{1} + i\mathbb{P}\Theta\mathbb{P}^{-1} + \frac{i\mathbb{P}\Theta\mathbb{P}^{-1}\, i\mathbb{P}\Theta\mathbb{P}^{-1}}{2!} + \dots$$

where we insert $\mathbb{P}^{-1}\mathbb{P} = \mathbb{1}$ between Θ's —

$$= \exp\{ i\mathbb{P}\Theta\mathbb{P}^{-1} \} \Rightarrow H = \mathbb{P}\Theta\mathbb{P}^{-1}$$

Now we need only prove that $\mathbb{P} \, \text{Ⓗ} \, \mathbb{P}^{-1}$ is Hermitian. The matrix Ⓗ is diagonal & related to H via a similarity transformation; so it consists of the eigenvalues. These eigenvalues are all real. If the eigenvalues of a matrix are real then -

$$(x, Hx) = (x, \lambda x) = (\lambda x, x) = (Hx, x)$$

thus H is Hermitian.

6 a) False – Let $\mathbb{A} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ $\mathbb{B} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

$\mathbb{A}\mathbb{B} = 0$, but $\mathbb{A}$ & $\mathbb{B} \neq 0$.

b) If all eigenvalues are the same then under a similarity transform –

$$\mathbb{D} = \mathbb{P}^{-1}\mathbb{A}\mathbb{P} = \begin{pmatrix} \lambda & & \tilde{0} \\ & \ddots & \\ \tilde{0} & & \lambda \end{pmatrix} = \lambda \mathbb{1}.$$

Then $\mathbb{A} = \mathbb{P}\mathbb{D}\mathbb{P}^{-1} = \mathbb{P}(\lambda\mathbb{1})\mathbb{P}^{-1}$

$= \lambda\mathbb{1}$

Thus $\mathbb{A}$ is always diagonal. (True!).

c) True – let $\mathbb{B} = \mathbb{A}^n$, with $\mathbb{A}^\dagger = \mathbb{A}$,

Then $\mathbb{B}^\dagger = (\mathbb{A}\mathbb{A}\cdots\mathbb{A})^\dagger$

$= \mathbb{A}^\dagger\mathbb{A}^\dagger\cdots\mathbb{A}^\dagger = \mathbb{A}\cdots\mathbb{A} = \mathbb{A}^n = \mathbb{B}.$

Thus $\mathbb{B}$ is self adjoint.

d) $\det(\mathbb{A}+\mathbb{B}) = \det\mathbb{A} + \det\mathbb{B}$ is <u>FALSE</u>.

$\mathbb{A} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ $\mathbb{B} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ $\mathbb{C} = \mathbb{A}+\mathbb{B} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

$\det\mathbb{A} + \det\mathbb{B} = 0$

$\det(\mathbb{A}+\mathbb{B}) = \det\mathbb{C} = 1.$

e) If A & B are Hermitian — is AB Hermitian ?

False. — if $C = AB$, then

$$C^\dagger = (AB)^\dagger = B^\dagger A^\dagger = BA$$

Thus only if $AB = BA$ will C be Hermitian.

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

Not equal and $C^\dagger \neq C$.

f) $\mathrm{Tr}\, AB = \mathrm{Tr}\, A\, \mathrm{Tr}\, B$ for finite dimensional spaces. $\boxed{\text{False}}$ — (NxN matrix)

Let $A = \mathbb{1}$, B = any matrix.

$$\mathrm{Tr}\, AB = \mathrm{Tr}\, \mathbb{1} B = \mathrm{Tr}\, B$$

$$\mathrm{Tr}\, \mathbb{1}\, \mathrm{Tr}\, B = \cancel{1}\ \mathrm{Tr}\, B.$$

N

17 a) $\mathbb{P}_i$ is idempotent –

$$\mathbb{P}_i x = x_i (x, x_i)$$

$$\mathbb{P}_i \mathbb{P}_i x = P_i \, x_i (x, x_i)$$

$$= x_i (x_i, x_i)(x, x_i)$$

$$= x_i (x, x_i) = \mathbb{P}_i x$$

Thus $\mathbb{P}_i^2 x = \mathbb{P}_i x$. $\forall x$.

b) $$P_i P_j x = P_i \, x_j (x_j, x)$$

$$= x_i \underbrace{(x_i, x_j)}_{=0 \text{ for } i \neq j} (x_j, x)$$

c). $\mathbb{P}_i$ has no inverse.

$P_i x_j = 0$, even though $x_j \neq 0$,

Thus P_i has a null vector ∴ by

Theorem 3.7 $\mathbb{P}_i$ has no inverse.

d) Assume we have a basis $\{x_i\}$ – then

$$x = \sum \alpha_j x_j$$

and $$\sum P_i x = \sum_i \sum_j \alpha_j P_i x_j$$

$$= \sum_i \sum_j \alpha_j \, x_i (x_i, x_j)$$

$$= \sum \alpha_j x_j = x$$

Thus $\sum_i' \mathbb{P}_i x = x \Rightarrow \sum_i' P_i = \mathbb{1}$.

e) $(x, \mathbb{P}_i x) = \sum_j' \sum_k' (\alpha_j x_j, P_i \alpha_k x_k)$.

$$= \sum_j' \sum_k' \alpha_j^* \alpha_k (x_j, P_i x_k).$$

$$= \sum_j' \sum_k' \alpha_j^* \alpha_k \underbrace{(x_j, x_i)}_{\delta_{ij}} \underbrace{(x_i, x_k)}_{\delta_{ik}}.$$

$$= |\alpha_i|^2$$

$$(\mathbb{P}_i x, x) = \sum_j' \sum_k' (P_i \alpha_j x_j, \alpha_k x_k)$$

$$= \sum_j' \sum_k' \alpha_j^* \alpha_k (x_i, x_j)(x_i, x_k)$$

$$= |\alpha_i|^2$$

Thus $(x, \mathbb{P} x) = (\mathbb{P}^\dagger x, x) = (\mathbb{P} x, x)$.

$\Rightarrow \mathbb{P}^\dagger = \mathbb{P}$. QED —

f). Resolve x into $x = \sum' \alpha_i x_i$ where the x_i are eigenvectors of $\mathbb{A}$. Then

$$\mathbb{A} x = \mathbb{A} \sum' \alpha_i x_i = \sum' \alpha_i \epsilon_i x_i$$

Similarly $\sum \epsilon_i \mathbb{P}_i$ on x yields —

$$\sum_i \epsilon_i P_i x = \sum_i \sum_j \epsilon_i P_i \alpha_j x_j$$
$$= \sum_i \epsilon_i \alpha_i x_i$$

Thus the effect of $\sum_i \epsilon_i P_i$ is the same as A for all x $\Rightarrow$ the two are equivalent.

Homework 8, problem 4

Problem

Take the three vectors

```
In[440]:= v1 = {1, 1, 1};
          v2 = {1, 2, 3};
          v3 = {1, 2, 1};
```

And orthonormalize them via the Gram-Schmidt process

Answer

Set x1 equal to the normalized v1:

In[443]:= $c1 = \sqrt{v1.v1}$

Out[443]= $\sqrt{3}$

In[444]:= `x1 = v1 / c1`

Out[444]= $\left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}$

Subtract from v2 the component of x1 along v2

In[448]:= `temp2 = v2 - (x1.v2) x1`

Out[448]= $\{-1, 0, 1\}$

Normalize this and set x2 equal to it:

In[449]:= $c2 = \sqrt{temp2.temp2}$

Out[449]= $\sqrt{2}$

In[450]:= `x2 = temp2 / c2`

Out[450]= $\left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}$

Subtract from v4 the components of x1 and x2 along v3

In[451]:= `temp3 = v3 - (x1.v3) x1 - (x2.v3) x2`

Out[451]= $\left\{-\frac{1}{3}, \frac{2}{3}, -\frac{1}{3}\right\}$

Normalize this and set x3 equal to it:

In[453]:=
```
c3 = Sqrt[temp3.temp3]
```

Out[453]= $\sqrt{\frac{2}{3}}$

In[454]:=
```
x3 = temp3 / c3
```

Out[454]= $\left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}$

Our three vectors are:

In[462]:=
```
MatrixForm[{{x1, x2, x3}}]
```

Out[462]//MatrixForm=

$$\begin{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix} & \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} & \begin{pmatrix} -\frac{1}{\sqrt{6}} \\ \sqrt{\frac{2}{3}} \\ -\frac{1}{\sqrt{6}} \end{pmatrix} \end{pmatrix}$$

Check :

In[457]:=
```
x1.x1 == x2.x2 == x3.x3 == 1
```

Out[457]= True

In[458]:=
```
x1.x2 == x2.x3 == x3.x1 == 0
```

Out[458]= True

There is always the quick way:

In[459]:=
```
Orthogonalize[{v1, v2, v3}]
```

Out[459]= $\left\{\left\{\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}, \left\{-\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right\}, \left\{-\frac{1}{\sqrt{6}}, \sqrt{\frac{2}{3}}, -\frac{1}{\sqrt{6}}\right\}\right\}$

5. Spinors!

(a) Show that

$$(\hat{\sigma}\cdot\hat{n})^k = 1 \quad \text{if } k \text{ is even.}$$

$$= \hat{\sigma}\cdot\hat{n} \quad \text{if } k \text{ is odd}$$

Trivially the second is true if we prove the first because if $k = 2n+1$ is odd then

$$(\hat{\sigma}\cdot\hat{n})^k = (\hat{\sigma}\cdot\hat{n})^{2p+1}$$

$$= (\hat{\sigma}\cdot\hat{n})^{2p}(\hat{\sigma}\cdot\hat{n}) =$$

$$1\,(\hat{\sigma}\cdot\hat{n}) = (\hat{\sigma}\cdot\hat{n})$$

To prove the first note that for $k=2$

$$(\hat{n}\cdot\hat{\sigma})(\hat{n}\cdot\hat{\sigma})$$

$$= (n_x\hat{\sigma}_x + n_y\hat{\sigma}_y + n_z\hat{\sigma}_z)\cdot(n_x\hat{\sigma}_x + n_y\sigma_y + n_z\sigma_z)$$

$$= n_x^2\hat{\sigma}_x^2 + n_y^2\hat{\sigma}_y^2 + n_z\hat{\sigma}_z^2$$

$$+ n_x n_y(\hat{\sigma}_x\hat{\sigma}_y + \hat{\sigma}_y\hat{\sigma}_x)$$

$$+ n_y n_z(\hat{\sigma}_y\hat{\sigma}_z + \hat{\sigma}_z\sigma_y)$$

$$+ n_z n_x(\hat{\sigma}_z\hat{\sigma}_y + \hat{\sigma}_y\hat{\sigma}_z)$$

For the Pauli matrices -

$$\hat{\sigma}_i\hat{\sigma}_j + \hat{\sigma}_j\hat{\sigma}_i = 2\delta_{ij}\,\mathbb{I}$$

$$(\hat{n}\cdot\hat{\sigma})^2 = (n_x^2 + n_y^2 + n_z^2)\,\mathbb{1} = \mathbb{1}$$

Then for any even power $k = 2p$

$$(\hat{n}\cdot\hat{\sigma})^k = \left[(\hat{n}\cdot\hat{\sigma})^2\right]^p = \mathbb{1}$$

(b) What is $\exp\left\{-i\,\frac{\hat{\sigma}\cdot\hat{n}\,\Delta\phi}{2}\right\}$?

This is the power series -

$$R(\Delta\phi) = 1 - i\,(\hat{\sigma}\cdot\hat{n})\,\frac{\Delta\phi}{2} + \frac{(-i)^2}{2!}(\hat{\sigma}\cdot\hat{n})^2\left(\frac{\Delta\phi}{2}\right)^2$$

$$+ \frac{1}{3!}(-i)^3(\hat{\sigma}\cdot\hat{n})^3\left(\frac{\Delta\phi}{2}\right)^3 + \frac{1}{4!}(-i)^4(\hat{\sigma}\cdot\hat{n})^4 + \cdots$$

$$= \left\{1 - \frac{1}{2!}\left(\frac{\Delta\phi}{2}\right)^2 + \frac{1}{4!}\left(\frac{\Delta\phi}{2}\right)^4 + \cdots\right\}$$

$$+ -i\,(\hat{\sigma}\cdot\hat{n})\left\{\frac{\Delta\phi}{2} - \frac{1}{3!}\left(\frac{\Delta\phi}{2}\right)^3 + \frac{1}{5!}\left(\frac{\Delta\phi}{2}\right)^5 - \cdots\right\}$$

$$= \cos\frac{\Delta\phi}{2}\,\mathbb{1} - i\,(\hat{\sigma}\cdot\hat{n})\sin\frac{\Delta\phi}{2}$$

(c) $$\cos\frac{\Delta\phi}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} - i\left\{n_x\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right.$$

$$\left. + n_y\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} + n_z\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right\}\sin\frac{\Delta\phi}{2}$$

$$= \begin{pmatrix} \cos\frac{\Delta\phi}{2} - i n_z \sin\frac{\Delta\phi}{2} & (-i n_x - n_y)\sin\frac{\Delta\phi}{2} \\ (-i n_x + n_y)\sin\frac{\Delta\phi}{2} & \cos\frac{\Delta\phi}{2} + i n_z \sin\frac{\Delta\phi}{2}. \end{pmatrix}$$

(d) Starting with $\begin{pmatrix}1\\0\end{pmatrix}$

i, $\frac{\pi}{2}$ about x-axis ⇒

$$n_x = 1 \;;\; n_y = n_z = 0$$

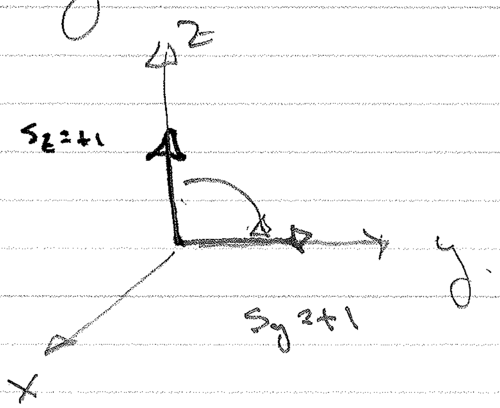
$$\mathbb{R}|\uparrow\rangle = \begin{pmatrix} \frac{1}{\sqrt2} & -\frac{i}{\sqrt2} \\ \frac{i}{\sqrt2} & \frac{1}{\sqrt2} \end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt2}\begin{pmatrix}1\\i\end{pmatrix}$$

This is $S_y = +1$

$$\hat\sigma_y \frac{1}{\sqrt2}\begin{pmatrix}1\\i\end{pmatrix} = \frac{1}{\sqrt2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}1\\i\end{pmatrix} = \frac{1}{\sqrt2}\begin{pmatrix}1\\i\end{pmatrix}$$

So it is an eigenvector of $\hat\sigma_y$ with eigenvalue +1

This makes geometric sense!



ii. Rotate by π about x-axis -

$$R|\uparrow\rangle = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -i \end{pmatrix}$$

$$= -i \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -i\,|\downarrow\rangle$$

So it now points down, up to a phase.

iii. Rotate by 2π -

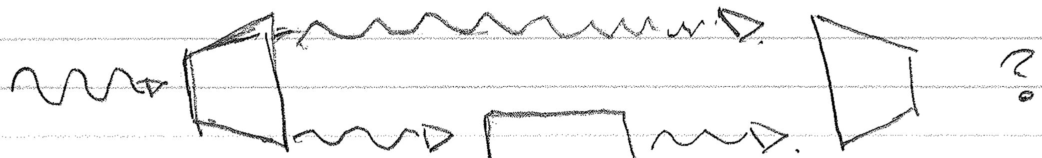
$$R|\uparrow\rangle = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \end{pmatrix}$$

$$= -|\uparrow\rangle$$

So rotating by 2π introduces a factor of (-1). This is a phase change & not a flip of the spin. However this is a strange feature of spin $\frac{1}{2}$ particles - to return them to their original state you must rotate them by 4π.

This is observable. If you have a beam

splitter & a field to rotate spin by 2π.



split rotate spin by 2π combine

With spin $\frac{1}{2}$ particles we get total <u>destructive</u> interference.

(e) No - rotating it by 2π is <u>not</u> the identity transformation -

"A spinor is an object that transforms as a spinor. A spin $\frac{1}{2}$ ket is <u>not</u> a 2-vector."

HW#8 Solutions:

Problem 6

(a) Normalization

Here's the wave function:

$$\text{psi} = \sqrt{\frac{2\,a^3}{\pi}}\,\frac{1}{x^2 + a^2};$$

Check normalization

```
Integrate[psi * psi, {x, -Infinity, Infinity}, GenerateConditions → False]
```

$$\sqrt{\frac{1}{a^2}}\; a$$

Mathematica can be finicky about whether constants are real or not. Let's force simplification:

```
PowerExpand[
 Integrate[psi * psi, {x, -Infinity, Infinity}, GenerateConditions → False]]
```

1

(b) Evaluation of energy:

```
k1 = -psi D[psi, x, x] // FullSimplify
```

$$\frac{4\,a^3\,\left(a^2 - 3\,x^2\right)}{\pi\,\left(a^2 + x^2\right)^4}$$

$$\text{v1} = -\frac{\text{psi} * \text{psi}}{1 + x^2}$$

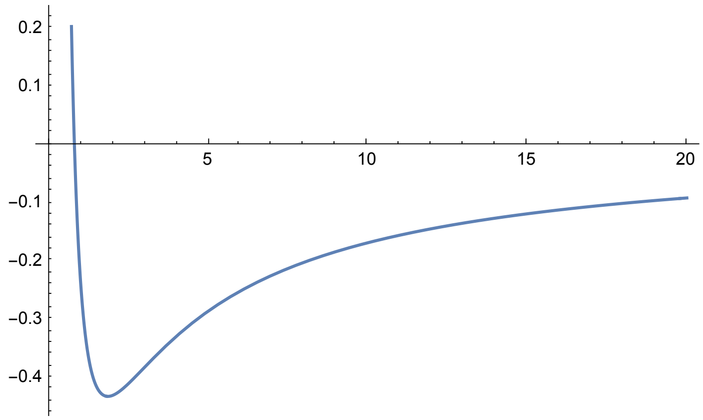
$$-\frac{2\,a^3}{\pi\,\left(1 + x^2\right)\,\left(a^2 + x^2\right)^2}$$

```
foo = PowerExpand[
   Integrate[k1 + v1, {x, -Infinity, Infinity}, GenerateConditions → False]]
```

$$\frac{1 - 4\,a^2 + 7\,a^4 - 4\,a^5}{2\,a^2\,\left(-1 + a^2\right)^2}$$

(c) Find the minimum:

```
Plot[foo, {a, 0, 20}]
```



Here are the solutions to when the derivative is zero.

```
soln = Solve[D[foo, a] == 0, a]
```

$$\left\{\left\{a \to -\frac{1}{2}\right\}, \left\{a \to \frac{1}{3} \times \left(1 + \left(19 - 3\sqrt{33}\right)^{1/3} + \left(19 + 3\sqrt{33}\right)^{1/3}\right)\right\},\right.$$
$$\left\{a \to \frac{1}{3} - \frac{1}{6} \times \left(1 + i\sqrt{3}\right)\left(19 - 3\sqrt{33}\right)^{1/3} - \frac{1}{6} \times \left(1 - i\sqrt{3}\right)\left(19 + 3\sqrt{33}\right)^{1/3}\right\},$$
$$\left.\left\{a \to \frac{1}{3} - \frac{1}{6} \times \left(1 - i\sqrt{3}\right)\left(19 - 3\sqrt{33}\right)^{1/3} - \frac{1}{6} \times \left(1 + i\sqrt{3}\right)\left(19 + 3\sqrt{33}\right)^{1/3}\right\}\right\}$$

Which one do we choose? Which one is physical? Let’s evalute these as numbers:

```
N[soln]
```

```
{{a → -0.5}, {a → 1.83929}, {a → -0.419643 + 0.606291 i}, {a → -0.419643 - 0.606291 i}}
```

Only the second answer is reasonable.

```
N[foo /. soln[[2]] ]
```

```
-0.432558
```

(d) Numerical solution

Set up mesh

```
xmax = 12.0;
npts = 200;
dx = 2 * xmax / (npts - 1)
```

```
0.120603
```

Create matrix

```
hmat = Table[0, {i, 1, npts}, {j, 1, npts}];
```

Poke in correct values of H:

```
Do[xj = -xmax + dx * (j - 1);
 hmat[[j, j]] = 2/(dx * dx) - 1/(1 + xj^2);, {j, 1, npts}]
Do[hmat[[j, j + 1]] = -1/(dx * dx);
 hmat[[j + 1, j]] = -1/(dx * dx);, {j, 1, npts - 1}]
```

```
eout = Eigensystem[hmat];
```

```
evals = eout[[1]]
```

```
{274.905, 274.902, 274.693, 274.67, 274.393, 274.313, 274.002, 273.829, 273.487,
 273.218, 272.834, 272.478, 272.042, 271.607, 271.114, 270.607, 270.053, 269.478,
 268.862, 268.22, 267.541, 266.834, 266.093, 265.322, 264.518, 263.685, 262.82,
 261.925, 260.998, 260.042, 259.056, 258.04, 256.995, 255.921, 254.817, 253.685,
 252.524, 251.336, 250.119, 248.875, 247.604, 246.305, 244.98, 243.629, 242.252,
 240.849, 239.421, 237.968, 236.491, 234.989, 233.464, 231.915, 230.342, 228.748,
 227.13, 225.491, 223.831, 222.149, 220.446, 218.724, 216.981, 215.219, 213.438,
 211.638, 209.821, 207.985, 206.132, 204.263, 202.377, 200.475, 198.558, 196.626,
 194.679, 192.719, 190.745, 188.757, 186.758, 184.746, 182.723, 180.688, 178.643,
 176.588, 174.524, 172.45, 170.368, 168.277, 166.179, 164.074, 161.963, 159.846,
 157.723, 155.595, 153.462, 151.326, 149.186, 147.044, 144.899, 142.752, 140.604,
 138.455, 136.306, 134.157, 132.009, 129.862, 127.717, 125.575, 123.435,
 121.299, 119.167, 117.039, 114.916, 112.798, 110.687, 108.582, 106.484,
 104.394, 102.311, 100.238, 98.1731, 96.118, 94.0731, 92.0387, 90.0153, 88.0036,
 86.0039, 84.0168, 82.0427, 80.0821, 78.1355, 76.2034, 74.2862, 72.3845,
 70.4986, 68.6291, 66.7763, 64.9408, 63.123, 61.3234, 59.5423, 57.7802, 56.0376,
 54.3149, 52.6124, 50.9307, 49.27, 47.6309, 46.0137, 44.4189, 42.8467, 41.2977,
 39.7721, 38.2704, 36.7929, 35.3399, 33.9119, 32.5091, 31.132, 29.7808, 28.456,
 27.1577, 25.8863, 24.6422, 23.4257, 22.2369, 21.0764, 19.9442, 18.8407,
 17.7661, 16.7209, 15.705, 14.719, 13.7628, 12.837, 11.9413, 11.0767, 10.2425,
 9.43985, 8.66785, 7.92814, 7.21901, 6.54305, 5.89736, 5.286, 4.70419, 4.15834,
 3.64067, 3.16133, 2.70787, 2.29622, 1.90682, 1.5643, 1.23866, 0.966991,
 0.705091, 0.506096, -0.438022, 0.309775, 0.184256, 0.0631009, 0.0039267}
```

```
Min[evals]
```

```
-0.438022
```

This is to be compared with the value above, -0.432. Note that the exact answer is lower in energy than the variational answer.

(e) Plot the eigenfunctions

Ok now let's find the eigenvector. To do so, we need to know it's place in the evecs array:

```
Position[evals, Min[evals]]
```

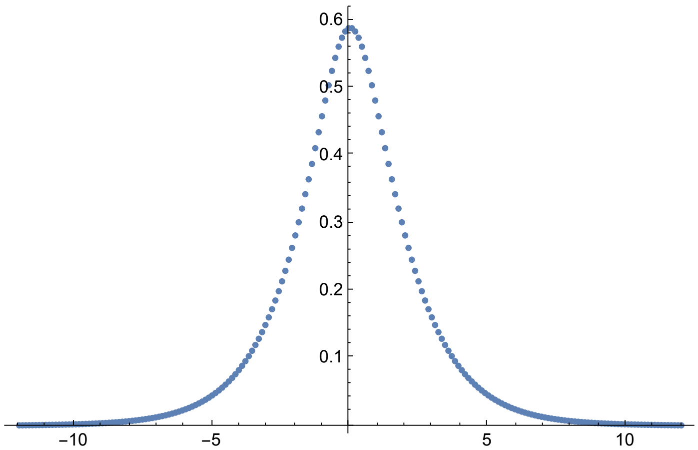
```
{{196}}
```

We want the 196th vector:

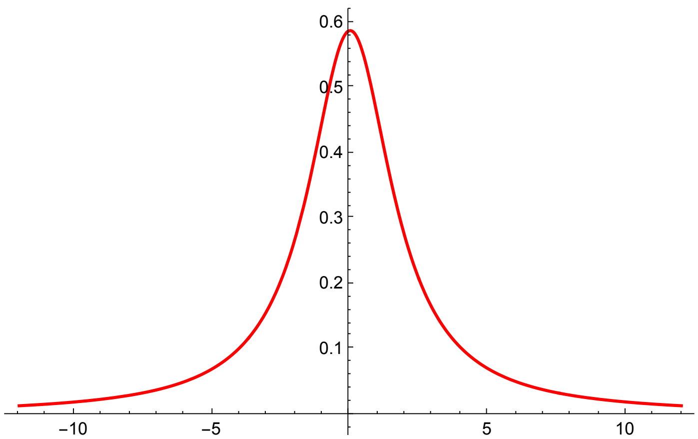
```
evecs = eout[[2]];
```

```
vecTemp = evecs[[196]];
numGS = vecTemp / (√(vecTemp.vecTemp * dx));
```

```
numGSplot = ListPlot[numGS, DataRange → {-12, 12}]
```




```
annGS = psi /. soln[[2]];
annGSplot = Plot[annGS, {x, -12, 12}, PlotStyle → Red]
```



```
Show[numGSplot, annGSplot]
```