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Math Methods in Physics

PHYS 5013 HOMEWORK ASSIGNMENT #8

PROBLEMS: $\{4.4, 4.6, 4.17, 4, 5, 6\}$

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Problem 1: 4.4

Let B be and $n \times n$ matrix. Define the $n \times n$ matrix $A = e^{iB}$ in terms of the power-series expansion exponential. That is,

$$A = \sum_{n=0}^{\infty} \frac{(iB)^n}{n!} = \mathbb{I} + iB + \frac{(iB)^2}{2!} + \cdots$$

Assuming that the series converges, prove that A is isometric if B is self-adjoint. Also show that any isometry U can be written as $U = \exp(iH)$, where H is Hermitian. Obtain an expression for H in terms of quantities related to U. [*Hint*: the properties of the eigenvectors and eigenvalues of the operators will be helpful.]

$$A = \sum_{n=0}^{\infty} \frac{(iB)^n}{n!} = \mathbb{1} + iB + \frac{(iB)^2}{2!} + \ldots\ldots, \quad A^{\dagger} = \sum_{n!} \frac{(iB)^n}{n!} = \mathbb{1} - iB^{\dagger} - \frac{(iB^{\dagger})}{2!} + \ldots\ldots$$

Isometric $\doteq$ $\mathcal{U}^{\dagger}\mathcal{U} = \mathbb{1}$ w/ $B = B^{\dagger}$,

$$A^{\dagger}A = \left(\mathbb{1} - iB^{\dagger} - \frac{(iB^{\dagger})^2}{2!} + \ldots\ldots\right)\left(\mathbb{1} + iB + \frac{(iB)^2}{2!} + \ldots\ldots\right)$$

$$= \mathbb{1} + \cancel{iB} + \cancel{\frac{(iB)^2}{2!}} - \cancel{iB^{\dagger}} + i\overset{0}{(\cancel{B^{\dagger}} - B)} - \cancel{iB^{\dagger}\frac{(iB)^2}{2!}} - \cancel{\frac{(iB^{\dagger})}{2!}} - \cancel{\frac{(iB^{\dagger})iB}{2!}} - \cancel{\frac{i^2(B^{\dagger} - B)^{0}}{(2!)}} = \mathbb{1}$$

A is isometric ✓

$A = \mathbb{1} + iB + \frac{(iB)^2}{2!} + \ldots\ldots$, w/ $H = B$, $\longrightarrow$ A is a power series expansion,

$A = \mathbb{1} + iH + \frac{(iH)}{2!} + \ldots\ldots$, $\text{Taylor}(e^x) = 1 + e^x + \frac{e^{2x}}{2!} + \ldots\ldots$ w/ $x = H = B$

we can write a finite version of A as

$$A = e^{iB} = e^{iH} \checkmark$$

$\mathcal{U} = S^{-1}DS$, w/ $D = e^{i\sigma_i}$ where σ_i are the eigenvalues of $\mathcal{U}$

$S\mathcal{U}S^{-1} = \mathbb{1} + i\sigma + \frac{(i\sigma)^2}{2!} \quad \therefore \quad \mathcal{U} = S^{-1}\left[\mathbb{1} + i\sigma + \frac{(i\sigma)^2}{2!}\right]S = \mathbb{1} + iS^{-1}\sigma S + \frac{i^2}{2}S^{-1}\sigma^2 S$

$\mathcal{U} = e^{iH} = \mathbb{1} + iH + \frac{(iH)^2}{2!} \quad \therefore \quad \mathbb{1} + iH + \frac{(iH)^2}{2!} = \mathbb{1} + iS^{-1}\sigma S + \frac{i^2}{2}S^{-1}\sigma^2 S \quad \therefore$

$$\boxed{H = S^{-1}\sigma S}$$

Problem 1: 4.4 Review

Procedure:

- Begin by expanding out $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{A}}^\dagger$ in the power series representation.
- Show that the $\tilde{\mathbf{A}}$ is isometric: i.e. $\tilde{\mathbf{A}}\tilde{\mathbf{A}}^\dagger = \mathbb{I}$.
- The isometry in turn shows us that $\tilde{\mathbf{B}}$ is self adjoint: i.e. $\tilde{\mathbf{B}} = \tilde{\mathbf{B}}^\dagger$.
- Show that $\tilde{\mathbf{A}}$ can be written in an exponential form.
- Use the relationship $\tilde{\mathbf{H}} = \tilde{\mathbf{S}}^{-1}\tilde{\mathbf{D}}\tilde{\mathbf{S}}$ where $\tilde{\mathbf{D}} = e^{i\theta_i}$ and θ_i are the eigenvalues of of $\tilde{\mathbf{H}}$.

Key Concepts:

- Isometry ($\tilde{\mathbf{U}}^\dagger\tilde{\mathbf{U}} = \mathbb{I}$) and unitary ($\tilde{\mathbf{U}}\tilde{\mathbf{U}}^\dagger = \mathbb{I}$) are not the same thing.
- An operator that is written in a power series can be expressed as an exponential.
- We use the relationship $\tilde{\mathbf{U}} = \tilde{\mathbf{S}}^{-1}\tilde{\mathbf{D}}\tilde{\mathbf{S}}$ to help find $\tilde{\mathbf{H}}$ in terms of related to $\tilde{\mathbf{U}}$.

Variations:

- We can be given a different operator for $\tilde{\mathbf{A}}$.
  - This would not change the process, but would slightly change the final answer from what we have now.
- We could be asked to show that the operator obeys different identities.
  - We would still expand the operator in a power series and then go about showing the other identities.

Problem 2: 4.6

Either prove or find a counterexample to the following statements:

(a) If A and B are $n \times n$ matrices, then $AB = 0$ implies that either $A = 0$ or $B = 0$.

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \text{ this is also } 0$$

(b) An $n \times n$ Hermitian matrix which is completely degenerate (all eigenvalues equal) is necessarily diagonal.

The only time this is true is if the matrix in question is if the matrix is a scalar multiple of the Identity:

$$(\lambda \hat{I})\vec{x} = \lambda \sum_{ij} |a_i\rangle\langle a_i| \hat{I} |a_j\rangle\langle a_j| \vec{x} = \lambda \sum_{ij} |a_i\rangle \underbrace{\langle a_i|a_j\rangle}_{\delta_{ij}} \langle a_j| \vec{x} = \lambda \sum_{i} |a_i\rangle\langle a_i| \vec{x} = \lambda \vec{x}$$

$\blacksquare$

(c) If an $n \times n$ matrix is Hermitian, then all its powers are Hermitian.

Hermitian matrix: $A = A^{+}$

For $n = 2$, $A^2 = AA = A^{+}A = AA^{+} = A^{+}A^{+} = (A^{+})^2 \quad \therefore \quad A^2 = (A^{+})^2$ or $A^n = (A^{+})^n$

$\blacksquare$

(d) $\det(A + B) = \det A + \det B$.

$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $B = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$, $A + B = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\det(A+B) = 1$: $\det(A) = 0$, $\det(B) = 0$

This is not true

(e) If A and B are $n \times n$ Hermitian matrices, then AB is Hermitian.

$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$: $\sigma_x \sigma_z = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, $\sigma_z \sigma_x = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, $\therefore \sigma_x \sigma_z \neq \sigma_z \sigma_x$

This is not true

(f) $\mathrm{tr}AB = \mathrm{tr}A\,\mathrm{tr}B$ in a finite-dimensional space.

$A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $B = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$: $\mathrm{Tr}(AB) = \mathrm{Tr}\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} = 4$, $\mathrm{Tr}(A)\mathrm{Tr}(B) = 2 \cdot 4 = 8$, $8 \neq 4 \; \therefore$

This is not true

Problem 2: 4.6 Review

Procedure:

- Begin by finding a trivial example that satisfies $AB = 0$.
- Show that for (b) the only time this is true is if the matrix in question is a scalar multiple of the identity matrix.
- Show that for Hermitian matrices are Hermitian regardless of the power of multiplication.
- Show that (d) - (f) are not true with trivial examples of matrices.

Key Concepts:

- Each part gives us a property that is true with matrices.
- The Pauli matrices are Hermitian.

Variations:

- We can be asked to prove different properties / identities.
  - Using the same properties and procedures we can show that they are either true or false.

Problem 3: 4.17

The projection operator P_i is defined as follows:

$$x' = P_i x \equiv x_i(x_i, x),$$

where x_i is a unit vector. This operator is called a projection operator because all x' are in the direction of x_i and the length of x' equals the component of x in the x_i direction, namely (x_i, x). In the following, let the x_i be a set of orthornormal vectors which span the n-dimensional vector space V. *Prove*:

(a) P_i is idempotent.

Idempotent : $P^2 = P$, $P = \sum_i |x_i\rangle\langle x_i|$, $P^2 = \sum_i |x_i\rangle\cancel{\langle x_i|x_i\rangle}^{1}\langle x_i| = \sum_i |x_i\rangle\langle x_i| = P$ ✓

■

(b) $P_i P_j = 0$ for $i \neq j$. Interpret geometrically.

$P_i = \sum_i |x_i\rangle\langle x_i|$, $P_j = \sum_j |x_j\rangle\langle x_j|$, $P_i P_j = \sum_i \sum_j |x_i\rangle\cancel{\langle x_i|x_j\rangle}^{0}\langle x_j| = 0$ $\therefore$ $P_i P_j = 0$

You cannot project a unit vector i, onto j since they are orthogonal

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(c) P_i has no inverse.

Since $P^2 = P$, the only possible matrix that can have an iverse and still satisfy $P^2 = P$ is $\mathbb{1}$.

$P^2 = P$, $PP = P$ if we have P^{-1}, $P \cdot P^{-1} \neq P$ unless $P = \mathbb{1}$

■

(d) $\sum_{i=1}^{n} P_i = \mathbb{I}$.

Take an arbitrary state $|\alpha\rangle$, $|\alpha\rangle = \sum_i |x_i\rangle\langle x_i|\alpha\rangle$, for $|\alpha\rangle = |\alpha\rangle$, $\sum_i |x_i\rangle\langle x_i| = \mathbb{1}$ ✓

■

(e) P_i is Hermitian.

For P_i to be Hermitian, $P_i = P_i^{+}$, if $P_i = \sum_i |x_i\rangle\langle x_i|$ then $P_i^{+} = \sum_i (|x_i\rangle\langle x_i|)^*$

Take $\langle\alpha|P_i^{+} = \sum_i \langle\alpha|x_i\rangle\langle x_i| = \sum_i c_i^* \langle x_i|$, $P_i|\alpha\rangle = \sum_i |x_i\rangle\langle x_i|\alpha\rangle = \sum_i c_i |x_i\rangle$

Since $\langle\alpha|\alpha\rangle = 1$, $\langle\alpha|P_i^{+}P_i|\alpha\rangle = \sum_i \langle\alpha|x_i\rangle\cancel{\langle x_i|x_i\rangle}^{1}\langle x_i|\alpha\rangle = \sum_i \cancel{\langle\alpha|x_i\rangle\langle x_i|\alpha\rangle}^{1} = \cancel{\langle\alpha|\alpha\rangle}^{1}$ ✓

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(f) Let A be a self-adjoint linear operator defined on an n-dimensional vector space V with n-eigenvalues, ϵ_i, and n-eigenvectors, x_i. Prove that A may be written as

$$A = \sum_{i=1}^{n} \epsilon_i P_i,$$

where P_i is as defined above. This is known as the spectral theorem for self-adjoint linear operators. (The analogous theorem for normal operators can also be easily proved.) Note the consistency of this result with parts (d) and (e) of this problem.

If A is self-adjoint, $(Ax_i, x_j) = (x_i, Ax_j)$

Problem 3: 4.17 Continued

Because A is self adjoint, this means $\epsilon_i = \epsilon_i^*$. Using parts (d) and (e),

$$A = \sum_i \epsilon_i |x_i\rangle\langle x_i| \quad , \quad A^\dagger = \sum_i \epsilon_i |x_i\rangle\langle x_i|$$

Since $P = P^\dagger$, we can deduce that this form is legitimate.

$\blacksquare$

Problem 3: 4.17 Review

Procedure:

- Show that x' is idempotent by expanding in a complete set.
- Show that $P_i P_j = 0$ by expanding in a complete set in i and in j, showing that the inner product of i and j will be zero.
- Demonstrate that it is impossible for P_i to have an inverse unless $P_i = \mathbb{I}$.
- Use an arbitrary state $|\alpha\rangle$ and expand in a complete set to show that for $|\alpha\rangle = |\alpha\rangle$, P_i must be an identity matrix.
- Expand P_i in a complete set, along with $P_i^\dagger$. Apply an arbitrary state and show that $P_i = P_i^\dagger$ and therefore Hermitian.
- With A being self adjoint, this means $\epsilon_i = \epsilon_i^\dagger$ and therefore with the prior properties it is proper to say that this form is legitimate.

Key Concepts:

- Idempotent means $P^2 = P$.
- Projection operators of the form P_i and P_j are orthogonal.
- Projection operators cannot have an inverse unless the projection operator is $\mathbb{I}$.
- We can use arbitrary states to prove a lot of identities that are asked of us to prove.
- Projection operators are Hermitian.
- Self adjoint means $\epsilon = \epsilon^\dagger$.

Variations:

- Since these are common properties of projection operators, this problem cannot be changed that much.
  - The form of which this is presented could be different but the same properties would hold.

Problem 4:

Consider the three vectors

$$\vec{v_1} = \hat{i} + \hat{j} + \hat{k}$$
$$\vec{v_2} = \hat{i} + 2\hat{j} + 3\hat{k}$$
$$\vec{v_3} = \hat{i} + 2\hat{j} + \hat{k}$$

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.

$\vec{V}_1 = (1,1,1)$, $\vec{V}_2 = (1,2,3)$, $\vec{V}_3 = (1,2,1)$: Let $\vec{u}_1, \vec{u}_2, \vec{u}_3$ be our $\perp$ vectors

Gram-Schmidt : $\vec{V}_1 = \vec{u}_1$, $\vec{u}_2 = \vec{V}_2 - \dfrac{\langle \vec{V}_2, \vec{V}_1 \rangle}{|\vec{V}_1|^2} V_1$, $\vec{u}_3 = \vec{V}_3 - \dfrac{\langle \vec{V}_3, \vec{V}_1 \rangle}{|\vec{V}_1|^2} \vec{V}_1 - \dfrac{\langle \vec{V}_3, \vec{u}_2 \rangle}{|\vec{u}_2|^2} \vec{u}_2$

$$\vec{u}_2 = (1,2,3) - \frac{(1,2,3)\cdot(1,1,1)}{(1,1,1)^2}(1,1,1) = (1,2,3) - \frac{6}{3}(1,1,1) = (1,2,3) - (2,2,2) = (-1,0,1)$$

$$\vec{u}_3 = (1,2,1) - \frac{(1,2,1)\cdot(1,1,1)}{(1,1,1)^2}(1,1,1) - \cancelto{0}{\frac{(1,2,1)\cdot(-1,0,1)}{(-1,0,1)^2}}(-1,0,1) = (1,2,1) - \frac{4}{3}(1,1,1) = \frac{1}{3}(-1,2,-1)$$

$$\hat{e}_i = \frac{\vec{V}_i}{|\vec{V}_i|} , \quad \hat{e}_1 = \frac{1}{\sqrt{3}}(1,1,1) , \quad \hat{e}_2 = \frac{1}{\sqrt{2}}(-1,0,1) , \quad \hat{e}_3 = \frac{1}{\sqrt{6}}(-1,2,-1)$$

$$\boxed{\hat{e}_1 = \frac{1}{\sqrt{3}}(1,1,1) , \quad \hat{e}_2 = \frac{1}{\sqrt{2}}(-1,0,1) , \quad \hat{e}_3 = \frac{1}{\sqrt{6}}(-1,2,-1)}$$

Problem 4: Review

Procedure:

- With $\vec{u}_1, \vec{u}_2, \vec{u}_3$ as our desired normalized vectors, and $\vec{v}_1$ as our first basis vector, use the following equations

$$\vec{u}_1 = \vec{v}_1, \quad \vec{u}_2 = \vec{v}_2 - \frac{\langle \vec{v}_2, \vec{v}_1 \rangle}{|\vec{v}_1|^2}\vec{v}_1, \quad \vec{u}_3 = \vec{v}_3 - \frac{\langle \vec{v}_3, \vec{v}_1 \rangle}{|\vec{v}_1|^2}\vec{v}_1 - \frac{\langle \vec{v}_3, \vec{u}_2 \rangle}{|\vec{u}_2|^2}\vec{u}_2.$$

- Take the results for $\vec{u}_1, \vec{u}_2, \vec{u}_3$ and normalize them.

Key Concepts:

- We can create orthonormalized vectors with the Gram-Schmidt process.
- These created vectors will all be orthogonal of one another while being normalized.

Variations:

- We can be given different vectors.
  - Thus giving us different values with the same procedure.
- We can have a different first basis vector.
  - This would change what we stick in for $\vec{v}_1$ in the above equation.

Problem 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 $\hat{\mathcal{T}} \equiv e^{\alpha \partial_x}$ is the *translation operator*, in that

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

In quantum mechanics this is written as:

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

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 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 $\triangle\phi$ one can use the operator

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

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:

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

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 be along the z-axis, with basis states:

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

(a) Show that

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

$$\sigma\cdot n = \sigma_x n_x + \sigma_y n_y + \sigma_z n_z, \quad (\sigma\cdot n)^k = (\sigma_x n_x + \sigma_y n_y + \sigma_z n_z)^k$$

$$= (\sigma_x n_x)^k + (\sigma_y n_y)^k + (\sigma_z n_z)^k + (n_x n_z\{\sigma_x, \sigma_z\})^k + (n_y n_z\{\sigma_y, \sigma_z\})^k + (n_x n_z\{\sigma_x, \sigma_z\})^k$$

$$\{\sigma_x, \sigma_z\} = \{\sigma_y, \sigma_z\} = \{\sigma_x, \sigma_z\} = 0 \quad \therefore \text{ Above} = (\sigma_x n_x)^k + (\sigma_y n_y)^k + (\sigma_z n_z)^k$$

$$(\sigma_x n_x)^k + (\sigma_y n_y)^k + (\sigma_z n_z)^k, \text{ w/ } \sqrt[k]{n_x^k + n_y^k + n_z^k} = 1, \quad \sigma_x^k + \sigma_y^k + \sigma_z^k = \mathbb{1} \text{ for k even}$$

$$\therefore (\sigma\cdot n)^k = \mathbb{1} \text{ for k even}$$

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$$(\sigma\cdot n)^{k\text{ odd}} = (\sigma\cdot n)^{k\text{ even}}\cdot(\sigma\cdot n) \quad \text{w/ } (\sigma\cdot n)^{k\text{ even}} = \mathbb{1}, \quad (\sigma\cdot n)^{k\text{ odd}} = (\sigma\cdot n)\mathbb{1}$$

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

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

$$e^{-i(\hat{\sigma}\cdot\hat{n})\Delta\varphi/2}, \quad \text{w/ } e^{-ix} = \sum_k \frac{(-i)^k x^k}{k!} \;:\; e^{-i(\hat{\sigma}\cdot\hat{n})\Delta\varphi/2} = \sum_k (-i)^k \frac{\left[(\hat{\sigma}\cdot\hat{n})\Delta\varphi/2\right]^k}{k!}$$

Problem 5: Continued

$$\sum_K (-i)^K \frac{[(\hat{\sigma}\cdot\hat{n})\Delta\varphi/2]^K}{K!} = \text{Even term} + \text{odd term} \Rightarrow \sum_K \frac{(-i)^K x^K}{K!} = \cos(x) - i\sin(x)$$

$$\sum_{K,\text{even}} (-i)^K \frac{[(\hat{\sigma}\cdot\hat{n})\Delta\varphi/2]^K}{K!} = \cos(\varphi/2) \quad , \quad \sum_{K,\text{odd}} (-i)^K \frac{[(\hat{\sigma}\cdot\hat{n})\Delta\varphi/2]^K}{K!} = -i\sin(\varphi/2)(\hat{\sigma}\cdot\hat{n})$$

$$(\hat{\sigma}\cdot\hat{n})^K = \mathbb{1} \text{ For even } K, \quad (\hat{\sigma}\cdot\hat{n})^K = \hat{\sigma}\cdot\hat{n} \text{ For odd } K$$

$$\therefore e^{-i(\hat{\sigma}\cdot\hat{n})\Delta\varphi/2} = \cos(\varphi/2) - i\sin(\varphi/2)(\hat{\sigma}\cdot\hat{n})$$

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(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:

$$\begin{pmatrix} \cos\frac{\phi}{2} - in_z\sin\phi/2 & (-in_x - n_y)\sin\frac{\phi}{2} \\ (-in_x + n_y)\sin\frac{\phi}{2} & \cos\frac{\phi}{2} + in_z\sin\phi/2 \end{pmatrix}$$

In general we have $R(\Delta\varphi)$ to be

$$R(\Delta\varphi) = \cos(\varphi/2)\mathbb{1} - i\sin(\varphi/2)(\hat{\sigma}\cdot\hat{n}) \quad , \quad \hat{\sigma}\cdot\hat{n} = n_x\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + n_y\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + n_z\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$R(\Delta\varphi) = \begin{pmatrix} \cos(\varphi/2) & 0 \\ 0 & \cos(\varphi/2) \end{pmatrix} - i\sin(\varphi/2)\begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix} \quad \therefore$$

$$R(\Delta\varphi) = \begin{pmatrix} \cos(\varphi/2) - in_z\sin(\varphi/2) & -i(n_x - in_y)\sin(\varphi/2) \\ -i(n_x + in_y)\sin(\varphi/2) & \cos(\varphi/2) + in_z\sin(\varphi/2) \end{pmatrix} \checkmark$$

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

(i) By $\pi/2$ about the ~~z~~ x-axis?

(ii) By π about the x-axis?

(iii) By $2/pi$ about the x-axis?

$$\boxed{R(\pi/2) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} , \quad R(\pi) = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} , \quad R(2\pi) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}}$$

$$\boxed{R(\pi/2)|\hat{\uparrow}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} , \quad R(\pi)|\hat{\uparrow}\rangle = \begin{pmatrix} 0 \\ -i \end{pmatrix} , \quad R(2\pi)|\hat{\uparrow}\rangle = \begin{pmatrix} -1 \\ 0 \end{pmatrix}}$$

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

$|\uparrow\rangle$ does not rotate as a vector due to the phase that it picks up in its rotation

Problem 5: Review

Procedure:

- Use the expanded form of $\sigma \cdot n$ to show that $(\sigma \cdot n)^k = \mathbb{I}$ when k is even.
- Use the prior result to show that $(\sigma \cdot n)^{k_{\text{odd}}} = (\sigma \cdot n)^{k_{\text{even}}}(\sigma \cdot n) = (\sigma \cdot n)\mathbb{I}$.
- Use the Euler identity along with a Taylor series expansion to collect the even and odd terms to prove the given result that is desired.
- For part (c), use the result in part (b) along with the Pauli matrices to prove that this rotation can be written in a matrix form.
- For a rotation about the x axis, set $n_y = n_z = 0$, and plug in the angle of which that is being rotated for ϕ.
- Identify that since the state $|\uparrow\rangle$ picks up a phase, it does not rotate like a vector.

Key Concepts:

- We can use the standard form for $\sigma \cdot n$ to prove the first identity in (a).
- We can write this rotation matrix in the form of an exponential or Taylor series expansion.
- We can then expand on the exponential form of this operator and write it as a matrix.
- For a rotation about the i^{th} axis, we set $n_i = 1$ and all other n's equal to 0. Then we can plug in the angle and the other value into the rotation matrix.
- When a rotation picks up a phase, this shows that the rotation will not behave like a vector.

Variations:

- Since this problem is asking us to prove identities more than anything, it can't be changed very much.
  - We can have different rotations of different axis', thus giving us different rotation matrices.
- We can be asked to rotate a different vector other than $|\uparrow\rangle$.
  - This could possibly show that the state does rotate like a vector as long as it does not pick up a phase.

Problem 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.

$$\int_{-\infty}^{+\infty} \psi^* \psi \, dx = \frac{2\alpha^3}{\pi} \int_{-\infty}^{+\infty} \frac{1}{(x^2+\alpha^2)^2} dx \cdot \frac{\cancel{2\alpha^3}}{\cancel{\pi}} \frac{\cancel{\pi}}{\cancel{2\alpha^3}} = 1 \checkmark, \quad \psi(x) \text{ is normalized}$$

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

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

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

$$\mathcal{L}(\alpha) = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}, \quad \langle \psi | \psi \rangle = 1, \quad \mathcal{L}(\alpha) = \frac{2\alpha^3}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2+\alpha^2} \left(-\frac{d^2}{dx^2} - \frac{1}{1+x^2} \right) \frac{1}{x^2+\alpha^2} dx$$

$$\mathcal{L}(\alpha) = \frac{2\alpha^3}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2+\alpha^2} \left(\frac{2}{(\alpha^2+x^2)^2} - \frac{8x^2}{(\alpha^2+x^2)^3} - \frac{1}{(1+x^2)(x^2+\alpha^2)} \right) dx$$

$$\mathcal{L}(\alpha) = \frac{2\alpha^3}{\pi} \int_{-\infty}^{+\infty} \frac{2}{(\alpha^2+x^2)^3} - \frac{8x^2}{(\alpha^2+x^2)^4} - \frac{1}{(1+x^2)(x^2+\alpha^2)^2} dx$$

$$\mathcal{L}(\alpha) = \frac{2\alpha^3}{\pi} \left[\int_{-\infty}^{+\infty} \frac{2}{(\alpha^2+x^2)^3} dx - \int_{-\infty}^{+\infty} \frac{8x^2}{(\alpha^2+x^2)^4} dx - \int_{-\infty}^{+\infty} \frac{1}{(1+x^2)(x^2+\alpha^2)^2} dx \right]$$

using mathematica and simplifying:

$$\boxed{\mathcal{L}(\alpha) = \frac{1}{2\alpha^2} - \frac{(1+2\alpha)}{(1+\alpha)^2}}$$

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

$$\frac{d}{d\alpha}\left(\frac{1}{2\alpha^2} - \frac{(1+2\alpha)}{(1+\alpha)^2} \right) = \frac{2\alpha}{(1+\alpha)^3} - \frac{1}{\alpha^3} = 0, \quad 2\alpha^4 = (1+\alpha)^3, \text{ using mathematica}$$

$$\boxed{\alpha = 1.839, \quad \mathcal{L}(1.839) = -0.432}$$

Problem 6: Continued

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

```
In[250]:= points = 2000;
dx = 7700.0/(points - 1);
mat = Table[0, {i, 1, points}, {j, 1, points}];
Do[mat[[i, i]] = -2/dx^2 - 1/(1 + (i dx - 3850.0)^2), {i, 1, points}];
Do[mat[[i, i + 1]] = -1/dx^2, {i, 1, points - 1}];
Do[mat[[i + 1, i]] = -1/dx^2, {i, 1, points - 1}];
evaluate = mat;
Min[Eigenvalues[evaluate]]

Out[257]= -0.432569
```

Problem 6: Review

Procedure

- Show that the state is normalized with
$$\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1.$$
- Calculate the expression for $\mathcal{L}$ using the Hamiltonian and state that is presented to us in the problem statement.
- Find the extrema of $\mathcal{L}$ and determine what value that gives for $\mathcal{L}$.
- Proceed to use the MATHEMATICA code in part (d) to find the ground state energy.

Key Concepts:

- We can find the ground state energy of a system with numerical methods.
- This ground state energy that is found in (d) should be the same that is found in (c).
- We find these values by having a variational form of the ground state, like the one that is given to us in the problem statement.

Variations:

- We can be given a different variational form of the ground state.
  - Thus changing the final values and expressions but not the overall process.
  - This is a consequence of having a different Hamiltonian than the one given in the problem statement.