Physics 143a – Workshop 12

Final Exam Review Problems

Problems

Note: All of these problems assume access to the final exam equation sheet.

1. **Time Evolution** (Adapted from [1])

   Suppose that the Hamiltonian is a linear operator with

   $$\hat{H}|\psi\rangle = \lambda|\phi\rangle, \quad \hat{H}|\phi\rangle = \lambda|\psi\rangle, \tag{1}$$

   where λ is an arbitrary real constant, and $|\psi\rangle$ and $|\phi\rangle$ are a pair of normalized independent (but **not** necessarily orthogonal) state vectors.

   (a) What are the conditions that $|\phi\rangle$ and $|\psi\rangle$ must satisfy in order for this Hamiltonian to be Hermitian?

   (b) With these conditions satisfied, find the states with definite energy and the corresponding energy values.

   (c) Say the system begins in the state $|\psi\rangle$. At what times is there zero probability to be found in the state $|\phi\rangle$?

2. **Harmonic oscillator** (Adapted from [2])

   Consider a one-dimensional harmonic oscillator of Hamiltonian $\hat{H}$ and stationary states $|n\rangle$:

   $$\hat{H}|n\rangle = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle, \tag{2}$$

   where $\hat{a}$ and $\hat{a}^\dagger$ are the raising and lowering operators of the harmonic oscillator satisfying $[\hat{a}, \hat{a}^\dagger] = 1$. The operator $\hat{U}(k)$ is defined by

   $$\hat{U}(k) = e^{ik\hat{X}}, \tag{3}$$

   where k is real and $\hat{X}$ is the position operator.

   (a) Is $\hat{U}(k)$ unitary? Show that for all n, its matrix elements satisfy the relation

   $$\sum_{n'}\left|\langle n|\hat{U}(k)|n'\rangle\right|^2 = 1. \tag{4}$$

   (b) Using the formula

   $$e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}}e^{\frac{1}{2}[\hat{A},\hat{B}]}, \tag{5}$$

   valid for $[\hat{A}, \hat{B}]$ commuting with $\hat{A}$ and $\hat{B}$, write $\hat{U}(k)$ as a product of exponential operators.

   (c) In terms of $E_k = \hbar^2k^2/2m$ and $E_\omega = \hbar\omega$, find an expression for the matrix element

   $$\langle n|\hat{U}(k)|0\rangle. \tag{6}$$

   (Note: $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ and $\hat{a}^\dagger|n\rangle = \sqrt{n}|n-1\rangle$)
   What happens as k approaches zero?

3. **Hydrogen Wave Function**

   You are told that the angular part of the electron's wave function in the hydrogen atom is

$$f(\theta, \phi) \propto \frac{1}{3} + (1 + \cos\phi \tan 2\theta) \cos 2\theta, \tag{7}$$

   where the proportionality constant is defined by normalization.

   (a) You measure the energy. What is the probability of finding the value -13.6 eV? What is the probability of finding the value -3.40 eV?

   (b) You measure $\mathbf{L}^2$. What values can you obtain and with what probabilities?

   (c) You measure L_z. What is the probability of obtaining the lowest L_z value?

4. **Spin vectors and density matrices** (Adapted from [3])

   (a) Consider a pure state of identically prepared spin $\frac{1}{2}$ systems. Suppose the expectation values $\langle S_x \rangle$ and $\langle S_z \rangle$ and the *sign* of $\langle S_y \rangle$ are known. How would we determine the state vector? Why is it unnecessary to know the magnitude of $\langle S_y \rangle$?

   (b) Consider a mixed state of spin $\frac{1}{2}$ systems. Suppose the mixed state averages $[S_x]$, $[S_y]$, and $[S_z]$ are all known. In terms of $[S_x]$, $[S_y]$, and $[S_z]$, write the inequality which defines this state as a mixed state.

Solutions

1. (a) In order for an operator to be Hermitian, it must be equal to its Hermitian conjugate. This in turn implies the operator has real eigenvalues and consequently real expectation values. Thus in order for $\hat{H}$ to be Hermitian, its expectation value must be real. With this condition, we have

$$\langle\psi|\hat{H}|\psi\rangle = \lambda\langle\psi|\phi\rangle = (\lambda\langle\psi|\phi\rangle)^* = \lambda\langle\phi|\psi\rangle, \tag{8}$$

where we used the fact that λ is real in the final equality. Computing $\langle\phi|\hat{H}|\phi\rangle$ produces a similar result, and so we see that in order for $\hat{H}$ to be hermitian, we need

$$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle. \tag{9}$$

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(b) Given Eq.(1), we find that $\hat{H}$ in the $|\psi\rangle$, $|\phi\rangle$ basis is

$$\hat{H} = \begin{pmatrix} \lambda\langle\psi|\phi\rangle & \lambda \\ \lambda & \lambda\langle\phi|\psi\rangle \end{pmatrix} \qquad [\text{in } |\psi\rangle, |\phi\rangle \text{ basis}]. \tag{10}$$

Computing the eigenvalues of this Hamiltonian, gives us

$$\begin{aligned} E_\pm &= \frac{\operatorname{Tr}\hat{H} \pm \sqrt{(\operatorname{Tr}\hat{H})^2 - 4\det\hat{H}}}{2} \\ &= \lambda\langle\phi|\psi\rangle \pm |\lambda| \end{aligned} \tag{11}$$

where we used $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle$. For simplicity, and without loss of generality, we will take $\lambda > 0$; The alternative choice $\lambda < 0$ can be analyzed similarly. For $\lambda > 0$, the eigenvalues become

$$E_\pm = \lambda\langle\phi|\psi\rangle \pm \lambda. \tag{12}$$

By inspection of Eq.(10) (or by solving the eigenvector equations), we find that the eigenvectors for Eq.(12) are

$$|E_+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad |E_-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \tag{13}$$

or, written explicitly in the $|\psi\rangle$, $|\phi\rangle$ basis, is

$$|E_+\rangle = \frac{1}{\sqrt{2}}|\psi\rangle + \frac{1}{\sqrt{2}}|\phi\rangle, \quad |E_-\rangle = \frac{1}{\sqrt{2}}|\psi\rangle - \frac{1}{\sqrt{2}}|\phi\rangle. \tag{14}$$

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(c) Since $\langle\phi|\psi\rangle \neq 0$, if the state begins in $|\psi\rangle$, there are no subsequent times at which there is zero probability to be in the state $|\phi\rangle$. We can see this by computing our time evolved state given the initial condition $|\alpha(t=0)\rangle = |\psi\rangle$. Applying the standard time-evolution operator, we find

$$\begin{aligned} |\alpha(t)\rangle &= e^{-i\hat{H}t/\hbar}|\psi\rangle \\ &= e^{-i\hat{H}t/\hbar}\left(\frac{1}{\sqrt{2}}|E_+\rangle + \frac{1}{\sqrt{2}}|E_-\rangle\right) \\ &= \frac{1}{\sqrt{2}}e^{-iE_+t/\hbar}|E_+\rangle + \frac{1}{\sqrt{2}}e^{-iE_-t/\hbar}|E_-\rangle. \end{aligned} \tag{15}$$

Computing the inner product between $|\alpha(t)\rangle$ and $|\phi\rangle$ yields the probability amplitude for the

$|\psi\rangle \to |\phi\rangle$ process:

$$\begin{aligned}\langle\phi|\alpha(t)\rangle &= \frac{1}{\sqrt{2}}e^{-iE_+t/\hbar}\langle\phi|E_+\rangle + \frac{1}{\sqrt{2}}e^{-iE_-t/\hbar}\langle\phi|E_-\rangle \\ &= \frac{1}{2}\left[(1+\langle\phi|\psi\rangle)e^{-iE_+t/\hbar} - (1-\langle\phi|\psi\rangle)e^{-iE_-t/\hbar}\right]. \end{aligned} \tag{16}$$

We want to find the times where $|\langle\phi|\alpha(t)\rangle|^2 = 0$. These times are equivalent to those for which $\langle\phi|\alpha(t)\rangle = 0$. Solving for these times using Eq.(16), we find

$$\frac{1+\langle\phi|\psi\rangle}{1-\langle\phi|\psi\rangle} = e^{-i(E_- - E_+)t/\hbar} = e^{-2i\lambda t/\hbar}. \tag{17}$$

Eq.(17) has no solution because while the right-hand side has modulus 1 for all t, the left hand side (given $\langle\phi|\psi\rangle \neq 0$) has a modulus which can never be 1. Therefore, we see that precisely because $|\phi\rangle$ and $|\psi\rangle$ are not orthogonal, if we begin in $|\psi\rangle$ there will always be a nonzero probability to be found in $|\phi\rangle$.

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2. (a) If k is real and $\hat{X}$ is Hermitian we find

$$\hat{U}(k)^\dagger = \exp\left(ik\hat{X}\right)^\dagger = \exp\left(-ik\hat{X}^\dagger\right) = \exp\left(-ik\hat{X}\right) \tag{18}$$

Therefore $\hat{U}\hat{U}^\dagger = e^{ik\hat{X}}e^{-ik\hat{X}} = \mathbb{I}$ and $\hat{U}$ is unitary.
Proving the stated identity, we have

$$\begin{aligned}\sum_{n'}\left|\langle n|\hat{U}(k)|n'\rangle\right|^2 &= \sum_{n'}\langle n|\hat{U}(k)|n'\rangle\langle n|\hat{U}(k)|n'\rangle^* \\ &= \sum_{n'}\langle n|\hat{U}(k)|n'\rangle\langle n|\hat{U}(k)|n'\rangle^\dagger \\ &= \sum_{n'}\langle n|\hat{U}(k)|n'\rangle\langle n'|\hat{U}(k)^\dagger|n\rangle \\ &= \langle n|\hat{U}(k)\left[\sum_{n'}|n'\rangle\langle n'|\right]\hat{U}(k)^\dagger|n\rangle \\ &= \langle n|\hat{U}(k)\mathbb{I}\,\hat{U}(k)^\dagger|n\rangle = \langle n|n\rangle = 1, \end{aligned} \tag{19}$$

where in the second line we used the fact that the Hermitian conjugate of a scalar is equivalent to the complex conjugate of the scalar.

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(b) Given the representation of $\hat{X}$ in terms of raising and lowering operators,

$$\hat{X} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^\dagger + \hat{a}\right), \tag{20}$$

the fact that $[\hat{a}, \hat{a}^\dagger] = 1$, and the identity $e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\frac{1}{2}[\hat{A},\hat{B}]}$ (for $[\hat{A},[\hat{A},\hat{B}]] = [\hat{B},[\hat{A},\hat{B}]] = 0$), we find

$$\begin{aligned}\hat{U}(k) &= \exp\left[iq\left(\hat{a}^\dagger + \hat{a}\right)\right] \\ &= \exp\left[iq\,\hat{a}^\dagger\right]\exp\left[iq\,\hat{a}\right]\exp\left[-\frac{1}{2}[iq\hat{a}^\dagger, iq\hat{a}]\right]\end{aligned}$$

$$= e^{iq\hat{a}^\dagger} e^{iq\hat{a}} e^{-q^2/2}, \tag{21}$$

where we defined $q \equiv k\sqrt{\frac{\hbar}{2m\omega}}$ for notational simplicity. As it expresses $\hat{U}(k)$ as a product of exponential operators, Eq.(21) is the desired result.

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(c) Given $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ and $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$, we can establish the identities

$$e^{iq\hat{a}}|0\rangle = |0\rangle \quad \text{and} \quad |m\rangle = \frac{(\hat{a}^\dagger)^m}{\sqrt{m!}}|0\rangle. \tag{22}$$

Now, calculating the matrix element $\langle n|\hat{U}(k)|0\rangle$, we find

$$\begin{aligned}
\langle n|\hat{U}(k)|0\rangle &= \langle n|e^{iq\hat{a}^\dagger} e^{iq\hat{a}}|0\rangle e^{-q^2/2} \\
&= \langle n|e^{iq\hat{a}^\dagger}|0\rangle e^{-q^2/2} \\
&= \langle n| \sum_{\ell=0}^{\infty} \frac{(iq)^\ell}{\ell!} (\hat{a}^\dagger)^\ell |0\rangle \, e^{-q^2/2} \\
&= \langle n| \sum_{\ell=0}^{\infty} \frac{(iq)^\ell}{\sqrt{\ell!}} |\ell\rangle \, e^{-q^2/2} \\
&= \frac{(iq)^n}{\sqrt{n!}} e^{-q^2/2}
\end{aligned} \tag{23}$$

where we used $\langle n|\ell\rangle = \delta_{n\ell}$ in the final line. Given that $E_k = \hbar^2 k^2/2m$ and $E_\omega = \hbar\omega$, we can write

$$q^2 = \frac{\hbar k^2}{2m\omega} = \frac{E_k}{E_\omega}. \tag{24}$$

Therefore, the computed matrix element is

$$\langle n|\hat{U}(k)|0\rangle = \frac{i^n}{\sqrt{n!}} \left(\frac{E_k}{E_\omega}\right)^{n/2} \exp\left[-\frac{E_k}{E_\omega}\right]. \tag{25}$$

We note that as $k \to 0$, $E_k \to 0$, and $\langle n|\hat{U}(k)|0\rangle \to 0$. This is consistent with the fact that $U(k) \to \mathbb{I}$ as $k \to 0$ and that $|n\rangle$ and $|0\rangle$ are orthonormal states.

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3. Before we complete the various parts of the problem, we must express $f(\theta, \phi)$ in terms of spherical harmonics. Employing various triogonometric identities, we find

$$\begin{aligned}
f(\theta, \phi) &\propto \frac{1}{3} + (1 + \cos\phi \tan 2\theta)\cos 2\theta \\
&= \frac{1}{3} + \cos 2\theta + \cos\phi \sin 2\theta \\
&= \frac{1}{3} + 2\cos^2\theta - 1 + 2\sin\theta\cos\theta\cos\phi \\
&= \frac{2}{3}\left(3\cos^2\theta - 1\right) + 2\sin\theta\cos\theta\cos\phi \\
&= \frac{2}{3}\sqrt{\frac{16\pi}{5}} Y_{2,0}(\theta,\phi) + \sqrt{\frac{8\pi}{15}}\Big[Y_{2,-1}(\theta,\phi) + Y_{2,+1}(\theta,\phi)\Big],
\end{aligned} \tag{26}$$

Because it will be relevant later, we normalize $f(\theta,\phi)$ by defining

$$f(\theta,\phi) = \frac{1}{\sqrt{N}}\left[\frac{2}{3}\sqrt{\frac{16\pi}{5}}Y_{2,0}(\theta,\phi) + \sqrt{\frac{8\pi}{15}}\Big[Y_{2,-1}(\theta,\phi) + Y_{2,+1}(\theta,\phi)\Big]\right], \tag{27}$$

where

$$N = \frac{4}{9}\times\frac{16\pi}{5} + 2\times\frac{8\pi}{15} = \frac{16\pi}{15}\times\frac{7}{3}. \tag{28}$$

(a) For the hydrogen atom, we have the energy spectrum $E_n = -13.6\text{ eV}/n^2$. Thus, energies of -13.6 eV and -3.4 eV correspond to the states $n = 1$ and $n = 2$, respectively. For the hydrogen atom wave functions, we know that values of ℓ for a given n can be $0,\ldots,n-1$. Thus, the $n = 1$ state can have $\ell = 0$, and the $n = 2$ state can have $\ell = 1$ or $\ell = 0$. None of these ℓ values are represented in Eq.(27) and thus the amplitudes for the corresponding n states are zero. Therefore, upon measuring the energy, the probability of finding -13.6 eV and the probability of finding -3.4 eV are both zero.

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(b) Because all of the spherical harmonics in Eq.(27) have $\ell = 2$, the only value of $\mathbf{L}^2$ we can obtain upon measurement is $\hbar^2 \times 2(2+1) = 6\hbar^2$. We obtain this value with 100% probability.

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(c) The probability of obtaining the lowest L_z value is the modulus squared of the third term in Eq.(27). Computing this result we find

$$\text{Prob}(L_z = -\hbar) = \frac{8\pi}{15}\times\frac{15}{16\pi} = \frac{3}{14}. \tag{29}$$

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4. (a) We know that an arbitrary normalized ket in the $|\pm\mathbf{z}\rangle$ basis can be written as

$$|\psi\rangle = \cos\frac{\theta}{2}|+\mathbf{z}\rangle + e^{i\phi}\sin\frac{\theta}{2}|-\mathbf{z}\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}, \tag{30}$$

where $\theta \in [0,\pi]$ and $\phi \in [0,2\pi]$. To fully determine the state we would need to determine the two parameters θ and ϕ. Given the following matrix representation of the spin $\frac{1}{2}$ operators

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{31}$$

and computing $\langle S_i\rangle = \langle\psi|\hat{S}_i|\psi\rangle$ with the matrix vector in Eq.(30), we find

$$\langle S_x\rangle = \frac{\hbar}{2}\sin\theta\cos\phi, \quad \langle S_y\rangle = \frac{\hbar}{2}\sin\theta\sin\phi, \quad \langle S_z\rangle = \frac{\hbar}{2}\cos\theta. \tag{32}$$

In the domain $\theta \in [0,\pi]$, the function $\cos\theta$ is one-to-one and is therefore invertible. So if we know the value of $\langle S_z\rangle$, we can determine θ with

$$\theta = \cos^{-1}\left(\frac{2\langle S_z\rangle}{\hbar}\right) \in [0,\pi]. \tag{33}$$

However, within the domain $\phi \in [0,2\pi]$, the function $\cos\phi$ is not one-to-one and is not invertible unless we restrict its domain. Specifically, given that $\sin x$ is only positive for $x \in [0,\pi]$, we know from Eq.(32) that $\langle S_y\rangle$ is positive when $\phi \in [0,\pi]$ and is negative when $\phi \in [\pi,2\pi]$.

Therefore, solving for ϕ using Eq.(33) and the first equation in Eq.(32), we find

$$\phi = \cos^{-1}\left(\frac{\langle S_x\rangle}{\sqrt{\hbar^2/4 - \langle S_z\rangle^2}}\right) \in \begin{cases} [0,\pi] & \text{if sgn}\,\langle S_y\rangle > 0 \\ [\pi, 2\pi] & \text{if sgn}\,\langle S_y\rangle < 0 \end{cases}. \tag{34}$$

The state Eq.(30) is then completely determined.

The reason we do not need to know the exact value of $\langle S_y\rangle$ is that Eq.(30) is defined by two parameters, and we only need two independent and invertible conditions to fully determine both parameters. With the values of both $\langle S_x\rangle$ and $\langle S_z\rangle$ known, we already have these two conditions, and knowing the sign of $\langle S_y\rangle$ ensures that the condition for $\langle S_x\rangle$ is invertible.

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(b) We want to find the inequality (written in terms of the ensemble averages of the spin operators) which defines the density operator $\hat{\rho}$ as a mixed state. We will first fully determine $\hat{\rho}$ and then compute the inequality.

The density matrix for an ensemble of spin $\frac{1}{2}$ states can be represented by a general 2×2 matrix with a trace of 1. For a general matrix $\hat{\rho}$, we have

$$\hat{\rho} = \begin{pmatrix} a_0 & a_1 \\ a_2 & a_3 \end{pmatrix}. \tag{35}$$

If we impose the condition that $\text{Tr}\,\hat{\rho} = 1$, we find the new matrix

$$\hat{\rho} = \begin{pmatrix} 1 - a_3 & a_1 \\ a_2 & a_3 \end{pmatrix}. \tag{36}$$

Calculating $[S_i] = \text{Tr}\,\hat{\rho}\hat{S}_i$ using Eq.(31) and Eq.(36), we find

$$[S_x] = \frac{\hbar}{2}(a_1 + a_2), \quad [S_y] = \frac{\hbar}{2}i(a_1 - a_2), \quad [S_z] = \frac{\hbar}{2}(1 - 2a_3), \tag{37}$$

which, when inverted, yields

$$a_1 = \frac{1}{\hbar}\left([S_x] - i[S_y]\right), \quad a_2 = \frac{1}{\hbar}\left([S_x] + i[S_y]\right), \quad a_3 = \frac{1}{2} - \frac{1}{\hbar}[S_z]. \tag{38}$$

Therefore, we can write Eq.(36) as

$$\hat{\rho} = \begin{pmatrix} \frac{1}{2} + \frac{1}{\hbar}[S_z] & \frac{1}{\hbar}\left([S_x] - i[S_y]\right) \\ \frac{1}{\hbar}\left([S_x] + i[S_y]\right) & \frac{1}{2} - \frac{1}{\hbar}[S_z] \end{pmatrix} = \frac{1}{2}\mathbb{I} + \frac{1}{\hbar}\left([S_x]\hat{\sigma}_1 + [S_y]\hat{\sigma_2} + [S_z]\hat{\sigma_3}\right), \tag{39}$$

where $\hat{\sigma_i}$ are the Pauli matrices. Now, if we have a mixed state, then $\hat{\rho}^2 \neq \hat{\rho}$ and, relatedly, $\hat{\rho}$ satisfies the inequality $\text{Tr}\,\hat{\rho}^2 < 1$. Given the Pauli matrix identity

$$\hat{\sigma}_i\hat{\sigma}_j + \hat{\sigma}_j\hat{\sigma}_i = 2\delta_{ij}\mathbb{I}, \tag{40}$$

(which can be established by direct calculation) and the fact that the Pauli matrices are traceless we find

$$\text{Tr}\,\hat{\rho}^2 = \text{Tr}\left[\frac{1}{4}\mathbb{I} + \frac{1}{\hbar^2}\left([S_x]^2 + [S_y]^2 + [S_z]^2\right)\mathbb{I}\right] = \frac{1}{2} + \frac{2}{\hbar^2}\left([S_x]^2 + [S_y]^2 + [S_z]^2\right). \tag{41}$$

Thus, given the mixed state inequality $\text{Tr}\,\hat{\rho}^2 < 1$, we have $[S_x]$, $[S_y]$, and $[S_z]$ are associated with a mixed state if they satisfy

$$[S_x]^2 + [S_y]^2 + [S_z]^2 < \frac{\hbar^2}{4}. \tag{42}$$

As a check we note the for the pure ensemble $\hat{\rho} = |+\mathbf{z}\rangle\langle+\mathbf{z}|$, $[S_y] = [S_x] = 0$ and $[S_z] = \hbar/2$, and the inequality in Eq.(42) becomes an equality.

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References

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[3] J. J. Sakurai, S.-F. Tuan, and E. D. Commins, "Modern quantum mechanics, revised edition," 1995.