

Some partial solutions and/or hints are given below.

As usual, there might be typos, so please use with care.

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1. A particle in a 1D harmonic oscillator: eigenstates.

For a single particle in a harmonic oscillator potential $V(x) = \frac{1}{2}m\omega^2 x^2$, the time-independent Schrodinger equation has an infinite number of eigenvalue/eigenfunction pairs. The lowest three energy eigenvalues are $E_0 = \frac{1}{2}\hbar\omega$, $E_1 = \frac{3}{2}\hbar\omega$, $E_2 = \frac{5}{2}\hbar\omega$. The corresponding eigenfunctions are respectively

$$\begin{aligned}\phi_0(x) &= A_0 e^{-x^2/2\sigma^2}, & \phi_1(x) &= A_1 x e^{-x^2/2\sigma^2}, \\ \phi_2(x) &= A_2 \left(\frac{2x^2}{\sigma^2} - 1 \right) e^{-x^2/2\sigma^2}. & \text{Here } \sigma^2 &= \frac{\hbar}{m\omega}.\end{aligned}$$

- (a) Sketch (by hand) plots of the three functions $\phi_n(x)$ for $n = 0$, $n = 1$, $n = 2$. You may use a computer program if you want to figure out how these functions look like, but please submit hand-drawn sketches. By looking at the three plots and observing the pattern, guess and sketch the plots of the next two eigenstates, $\phi_3(x)$ and $\phi_4(x)$.

Solution/Hints/Discussion →

As we increase n , the eigenfunctions have more and more 'nodes', i.e., zeros. The $n = 0$ case is the gaussian, which has no nodes. The next eigenfunctions have one, two, three, four,.... nodes.

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- (b) Look up (or calculate, or ask a computer algebra system or online integrator) the integrals

$$\int_{-\infty}^{+\infty} x^{2n} e^{-x^2} dx$$

for $n = 0$, $n = 1$, $n = 2$. Report the three results.

The first one ($n = 0$, integral over a Gaussian) is important enough that you might consider learning it for life. (You should certainly know how to derive it!)

Solution/Hints/Discussion →

$$\int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{\pi} \quad \int_{-\infty}^{+\infty} x^2 e^{-x^2} dx = \frac{\sqrt{\pi}}{2}$$

$$\int_{-\infty}^{+\infty} x^4 e^{-x^2} dx = \frac{3\sqrt{\pi}}{4}$$

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(c) Calculate the integrals

$$\int_{-\infty}^{+\infty} x^{2n} \exp\left[-\frac{x^2}{2\sigma^2}\right] dx$$

for $n = 0, n = 1, n = 2$, based on the results of the previous question.

Solution/Hints/Discussion →

You can calculate these through a variable substitution, say $u = x/(\sqrt{2}\sigma)$.

$$\int_{-\infty}^{+\infty} \exp\left[-\frac{x^2}{2\sigma^2}\right] dx = \sqrt{2\pi}\sigma$$

$$\int_{-\infty}^{+\infty} x^2 \exp\left[-\frac{x^2}{2\sigma^2}\right] dx = \sqrt{2\pi}\sigma^3$$

$$\int_{-\infty}^{+\infty} x^4 \exp\left[-\frac{x^2}{2\sigma^2}\right] dx = 3\sqrt{2\pi}\sigma^5$$

For the harmonic oscillator, one might also need the related integrals where the argument of the exponential is $-x^2/\sigma^2$ instead of $-x^2/(2\sigma^2)$. Hopefully, you can convince yourself that

$$\int_{-\infty}^{+\infty} \exp\left[-\frac{x^2}{\sigma^2}\right] dx = \sqrt{\pi}\sigma$$

$$\int_{-\infty}^{+\infty} x^2 \exp\left[-\frac{x^2}{\sigma^2}\right] dx = \frac{\sqrt{\pi}}{2}\sigma^3$$

$$\int_{-\infty}^{+\infty} x^4 \exp\left[-\frac{x^2}{\sigma^2}\right] dx = \frac{3\sqrt{\pi}}{4}\sigma^5$$

We will be using some of these later on.

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- (d) Use symmetry arguments to evaluate the integral

$$\int_{-\infty}^{+\infty} x^{2n+1} \exp\left[-\frac{x^2}{2\sigma^2}\right] dx$$

for any integer n . The integrand is an **odd** function.

Solution/Hints/Discussion →

ZERO

Why? If you plot the integrand for any integer n (try $n = 0$ or $n = 1$), you will find that area under the curve for positive x values (right half of your plot) is exactly canceled by the area under the curve for negative x values (left half of your plot). Hence the total integral is zero.

The integrand is an **odd** function of x , i.e., it has the form $f(-x) = -f(x)$. The integral of any odd function over $(-\infty, \infty)$ is zero, as the integral over $(-\infty, 0)$ cancels the integral over $(0, \infty)$.

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- (e) Show that ϕ_0 and ϕ_1 are orthogonal to each other, as are ϕ_1 and ϕ_2 , and finally that ϕ_0 and ϕ_2 are orthogonal to each other.

Solution/Hints/Discussion →

$\phi_0(x)\phi_1(x)$ is an odd function of x . Hence $\int_{-\infty}^{\infty} dx \phi_0(x)\phi_1(x) = 0$.

ϕ_1 and ϕ_2 are orthogonal for the same reason.

ϕ_0 and ϕ_2 : the integrand is not odd, so this needs more work:

$$\begin{aligned} \int_{-\infty}^{\infty} dx \phi_0(x)\phi_2(x) &= A_0 A_2 \int_{-\infty}^{\infty} dx e^{-x^2/2\sigma^2} \left(\frac{2x^2}{\sigma^2} - 1 \right) e^{-x^2/2\sigma^2} \\ &= A_0 A_2 \left[\frac{2}{\sigma^2} \int_{-\infty}^{\infty} dx x^2 e^{-x^2/2\sigma^2} - \int_{-\infty}^{\infty} dx e^{-x^2/2\sigma^2} \right] \\ &= A_0 A_2 \left[\frac{2}{\sigma^2} \left(\frac{\sqrt{\pi}}{2} \sigma^3 \right) - \sqrt{\pi} \sigma \right] = 0 \end{aligned}$$

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- (f) Show in general that, if $|w_1\rangle$ and $|w_2\rangle$ are eigenstates of a hermitian operator corresponding to distinct eigenvalues, then they are orthogonal to each other. (This is an important result.)

Solution/Hints/Discussion \rightarrow

Let the operator be \hat{A} , and the corresponding eigenvalues be a_1 and a_2 :

$$\hat{A}|w_1\rangle = a_1|w_1\rangle \quad \hat{A}|w_2\rangle = a_2|w_2\rangle$$

Since \hat{A} is hermitian, $\hat{A} = \hat{A}^\dagger$. Also, a_1 and a_2 are real. So, the first equation gives the dual relation:

$$\langle w_1|\hat{A}^\dagger = a_1^*\langle w_1| \quad \Longrightarrow \quad \langle w_1|\hat{A} = a_1\langle w_1|$$

Applying $\langle w_1|$ on the second eigenvalue equation:

$$\langle w_1|\hat{A}|w_2\rangle = \langle w_1|a_2|w_2\rangle \quad \Longrightarrow \quad a_1\langle w_1|w_2\rangle = a_2\langle w_1|w_2\rangle$$

Since $a_1 \neq a_2$, this implies $\langle w_1|w_2\rangle = 0$, i.e., that the two kets are orthogonal to each other.

This is really a very important result; please make sure you can reproduce the proof. E.g., using the fact that the Hamiltonian is hermitian, prove that eigenstates corresponding to different eigen-energies are orthogonal to each other.

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- (g) Calculate A_0 so that ϕ_0 is normalized.

Solution/Hints/Discussion \rightarrow

$$\int_{-\infty}^{\infty} dx |\phi_0(x)|^2 = |A_0|^2 \int_{-\infty}^{\infty} dx \exp\left[-\frac{x^2}{\sigma^2}\right] dx = |A_0|^2 \sqrt{\pi}\sigma$$

Normalization requires the norm above to be unity.

If you assume A_0 to be real and positive (why would you assume that?), then you would write

$$A_0 = \frac{1}{\sqrt{\sqrt{\pi\sigma}}} = \frac{1}{\pi^{1/4}\sigma^{1/2}}$$

Of course this is not general. If we want to avoid assuming that A_0 is real and positive, we can keep our result general with the help of a phase factor:

$$A_0 = \frac{e^{i\lambda}}{\pi^{1/4}\sigma^{1/2}} \quad \left\{ \begin{array}{l} \text{where } \lambda \text{ is an} \\ \text{arbitrary real number} \end{array} \right.$$

or we can just write the norm of A_0 and admit that we don't have a way to determine the phase or sign of A_0 :

$$|A_0| = \frac{1}{\sqrt{\sqrt{\pi\sigma}}} = \frac{1}{\pi^{1/4}\sigma^{1/2}}$$

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- (h) Calculate A_1 and A_2 so that ϕ_1 and ϕ_2 are normalized.

Solution/Hints/Discussion →

A_1 is calculated similarly:

$$|A_1| = \sqrt{\frac{2}{\sqrt{\pi\sigma}}} = \frac{\sqrt{2}}{\pi^{1/4}\sigma^{3/2}}$$

A_2 is calculated similarly as above, but much more tedious. I believe the answer should be

$$|A_2| = \sqrt{\frac{1}{\sqrt{\pi}2\sigma}} = \frac{1}{\pi^{1/4}(2\sigma)^{1/2}}$$

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- (i) Construct a solution of the TDSE, based on the three eigenfunctions of the time-independent SE.

Solution/Hints/Discussion →

The solutions of the TDSE corresponding to the three time-independent wavefunctions are

$$\begin{aligned}\phi_0(x)e^{-E_0t/\hbar} &= \phi_0(x)e^{-\frac{1}{2}\omega t} \\ \phi_1(x)e^{-E_1t/\hbar} &= \phi_1(x)e^{-\frac{3}{2}\omega t} \\ \phi_2(x)e^{-E_2t/\hbar} &= \phi_2(x)e^{-\frac{5}{2}\omega t}\end{aligned}$$

The general solution is

$$B\phi_0(x)e^{-\frac{1}{2}\omega_0t} + C\phi_1(x)e^{-\frac{3}{2}\omega_0t} + D\phi_2(x)e^{-\frac{5}{2}\omega_0t}$$

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- (j) At time $t = 0$, the particle in the harmonic oscillator finds itself in the state

$$\psi(x, 0) = \frac{1}{\sqrt{2}}\phi_0(x) - \frac{1}{2}\phi_1(x) + \frac{1}{2}\phi_2(x).$$

What is the wavefunction (state) $\psi(x, t)$ at a later time t ?

Solution/Hints/Discussion →

Comparing with the general solution written above, we see that the given initial state fixes the constants B, C, D . Thus the wavefunction at arbitrary later time is given by

$$\psi(x, t) = \frac{1}{\sqrt{2}}\phi_0(x)e^{-\frac{1}{2}\omega t} - \frac{1}{2}\phi_1(x)e^{-\frac{3}{2}\omega t} + \frac{1}{2}\phi_2(x)e^{-\frac{5}{2}\omega t}$$

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- (k) If the $\phi_n(x)$ functions are normalized, then show that $\psi(x, 0)$ is normalized, and that $\psi(x, t)$ remains normalized at later times t .

Solution/Hints/Discussion →

This is a very instructive exercise, which I leave for you to do.

You will also have to use the fact that the $\phi_n(x)$ functions are orthogonal to each other. You will not have to do any integrals.

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- (l) This is a good time to have a first browse through Nash Chapter 4 (The harmonic oscillator), or the wikipedia page on “Quantum Harmonic Oscillator”.
2. Let $|\phi_n\rangle$ be the orthonormalized energy eigenstate of a particle of mass m in an infinite square well of width a , with corresponding energy eigenvalue

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, \quad n = 1, 2, 3, \dots$$

The particle is prepared to be in the state

$$|\psi\rangle = \sum_{n=1}^{\infty} \frac{\alpha}{n^2} |\phi_n\rangle$$

where α is a positive real number.

- (a) You might need the series

$$\sum_{n=1}^{\infty} \frac{1}{n^4} = \frac{\pi^4}{90}, \quad \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}$$

Feel free to have fun deriving these two series sums.

Solution/Hints/Discussion →

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(b) Show that $|\psi\rangle$ is normalized if $\alpha = \sqrt{90/\pi^4}$.

Solution/Hints/Discussion \rightarrow

Since the $|\phi_n\rangle$ are orthonormalized,

$$\langle\phi_m|\phi_n\rangle = \delta_{mn}$$

The norm of the state $|\psi\rangle = \sum \frac{\alpha}{n^2}|\phi_n\rangle$ is therefore

$$\begin{aligned} \langle\psi|\psi\rangle &= \left(\sum_{n=1}^{\infty} \frac{\alpha^*}{n^2} \langle\phi_n|\right) \left(\sum_{n=1}^{\infty} \frac{\alpha}{n^2} |\phi_n\rangle\right) \\ &= \left(\sum_{l=1}^{\infty} \frac{\alpha^*}{l^2} \langle\phi_l|\right) \left(\sum_{n=1}^{\infty} \frac{\alpha}{n^2} |\phi_n\rangle\right) \quad \left\{ \begin{array}{l} \text{Changed a dummy variable} \\ \text{to avoid confusion} \end{array} \right. \\ &= \sum_{l=1}^{\infty} \sum_{n=1}^{\infty} \frac{\alpha^*}{l^2} \frac{\alpha}{n^2} \langle\phi_l|\phi_n\rangle = |\alpha|^2 \sum_{l=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{l^2} \frac{1}{n^2} \delta_{ln} \end{aligned}$$

If we perform the summation over n , only the term $n = l$ survives, by definition of the Kronecker delta δ_{ln} . Hence

$$\langle\psi|\psi\rangle = |\alpha|^2 \sum_{l=1}^{\infty} \frac{1}{l^2} \frac{1}{l^2} = |\alpha|^2 \sum_{l=1}^{\infty} \frac{1}{l^4} = |\alpha|^2 \frac{\pi^4}{90}$$

The result $\pi^4/90$ for the infinite series is given in the exam paper.

To be normalized, we require the norm to be 1; hence

$$|\alpha|^2 = \frac{90}{\pi^4} \quad \implies \quad \alpha = \frac{3\sqrt{10}}{\pi^2} \times \text{phase factor}$$

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(c) Find the expectation value of the Hamiltonian for this state.

Solution/Hints/Discussion \rightarrow

Since the $|\phi_n\rangle$ are energy eigenstates,

$$\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle \quad \langle\phi_l|\hat{H}|\phi_n\rangle = E_n\langle\phi_l|\phi_n\rangle = E_n\delta_{ln}$$

The expectation value of energy is

$$\begin{aligned}
 \langle \psi | \hat{H} | \psi \rangle &= \left(\sum_{n=1}^{\infty} \frac{\alpha^*}{n^2} \langle \phi_n | \right) \hat{H} \left(\sum_{n=1}^{\infty} \frac{\alpha}{n^2} | \phi_n \rangle \right) \\
 &= \left(\sum_{l=1}^{\infty} \frac{\alpha^*}{l^2} \langle \phi_l | \right) \hat{H} \left(\sum_{n=1}^{\infty} \frac{\alpha}{n^2} | \phi_n \rangle \right) \quad \left\{ \begin{array}{l} \text{using different summation variables} \\ \text{to avoid confusion} \end{array} \right. \\
 &= \sum_{l=1}^{\infty} \sum_{n=1}^{\infty} \frac{\alpha^*}{l^2} \frac{\alpha}{n^2} \langle \phi_l | \hat{H} | \phi_n \rangle = |\alpha|^2 \sum_{l=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{l^2} \frac{1}{n^2} E_n \delta_{ln} \\
 &= |\alpha|^2 \sum_{l=1}^{\infty} \frac{E_l}{l^4} = \frac{90}{\pi^4} \sum_{l=1}^{\infty} \frac{E_l}{l^4} = \frac{90}{\pi^4} \sum_{n=1}^{\infty} \frac{E_n}{n^4}
 \end{aligned}$$

Using $E_n = \frac{\pi^2 \hbar^2}{2ma^2} n^2$, we obtain

$$\langle \psi | \hat{H} | \psi \rangle = \frac{45 \hbar^2}{ma^2 \pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{45 \hbar^2}{ma^2 \pi^2} \frac{\pi^2}{6} = \frac{15 \hbar^2}{2ma^2}$$

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- (d) What is the probability that a measurement of the energy gives $2\pi^2 \hbar^2 / ma^2$, and if this energy is found, what state is the particle in immediately afterwards?

Hint: This question is about measurement in quantum mechanics. For guidance, you could try reading the first few sections of the wikipedia page on “Measurement in Quantum Mechanics”, and Sections 3.2 and 3.3 of Nash notes. There is also a paragraph summarizing measurement in the writeup “Essentials of QM”, linked on the webpage.

Solution/Hints/Discussion →

A measurement of energy results necessarily in one of the eigenvalues, E_n . The probability of finding the energy E_n , i.e., the probability of finding the system in the state $|\phi_n\rangle$, is $|\langle \phi_n | \psi \rangle|^2$. Equivalently, if the state $|\psi\rangle$ is expanded in the eigenstates $|\phi_n\rangle$, the mod-sqaure of the coefficient of $|\phi_j\rangle$ gives the probability of finding the energy to be E_j .

If the energy is found to be E_j , then the system will be in the state $|\phi_j\rangle$ immediately after the measurement.

A measurement of energy will give the result

$$\frac{2\pi^2\hbar^2}{ma^2} = \frac{\pi^2\hbar^2}{2ma^2}2^2 = E_2$$

with a probability $|\langle\phi_2|\psi\rangle|^2$. Noting that

$$\langle\phi_2|\psi\rangle = \langle\phi_2|\left(\sum_{n=1}^{\infty}\frac{\alpha}{n^2}|\phi_n\rangle\right) = \sum_{n=1}^{\infty}\frac{\alpha}{n^2}\langle\phi_2|\phi_n\rangle = \sum_{n=1}^{\infty}\frac{\alpha}{n^2}\delta_{2,n} = \frac{\alpha}{2^2}$$

we get for the probability

$$|\langle\phi_i|\psi\rangle|^2 = \frac{|\alpha|^2}{16} = \frac{1}{16}\frac{90}{\pi^4} = \frac{45}{8\pi^4} \approx 0.0577$$

If the energy is found to be E_2 , then the system will be in the state $|\phi_2\rangle$ immediately after the measurement.

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