Física Quântica I / Mecânica Quântica (2021/22)

Folha de Problemas 10 (Potencial delta Dirac. Oscilador harmónico 1D)

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— Soluções —

Problema 1 | Potencial delta de Dirac

Considere uma partícula de massa m sob influência do seguinte potencial (1D):

$$V(x) = -V_0 a\, \delta(x), \qquad (a, V_0 > 0)\,.$$

V_0 e a são constantes positivas com dimensões de energia e comprimento, respetivamente. $\delta(x)$ é a função delta de Dirac, a qual se anula em todo o eixo x, exceto na origem onde $\delta(0) = +\infty$.

1. Derive a condição fronteira que este potencial impõe na origem para a derivada da função de onda dos estados estacionários neste potencial. (*Integre a ESIT numa vizinhança infinitesimal desse ponto.*)

2. Mostre que este potencial tem um estado estacionário ligado com energia negativa. Calcule essa energia, E_0, e a função de onda respetiva, $\varphi_0(x)$, normalizada.

3. Se a partícula estiver no referido estado ligado, como se exprime a probabilidade de a encontrar na região do espaço $-a < x < a$ em termos dos parâmetros m, a e V_0?

4. Se o sinal de V_0 for invertido, quantos estados ligados podemos esperar para o potencial resultante?

5. Calcule os coeficientes de reflexão e transmissão em função da energia para o espalhamento de partículas com energia positiva pelo potencial original (com $V_0 > 0$).

Solution

1. The presence of a Dirac-delta potential creates a special situation, because the potential is strictly infinite at $x = 0$, but zero everywhere else. To understand what happens to the derivative of the wavefunction at this point, let us begin with the time-independent Schrödinger equation that we need to solve,

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\,\psi(x) = E\,\psi(x). \tag{1.1}$$

We now choose some arbitrary point $x = x_0$ and integrate this equation in the infinitesimal interval $(x_0 - \xi, x_0 + \xi)$ around the point x_0:

$$-\frac{\hbar^2}{2m}\int_{x_0-\xi}^{x_0+\xi} \psi''(x)\,dx + \int_{x_0-\xi}^{x_0+\xi} V(x)\,\psi(x)\,dx = E\int_{x_0-\xi}^{x_0+\xi} \psi(x)\,dx, \tag{1.2}$$

where $\xi \approx 0$ is an infinitesimal constant that we shall take to zero in the end. From basic calculus, we know that

$$\int_{x_0-\xi}^{x_0+\xi} \psi''(x)\, dx = \psi'(x_0+\xi) - \psi'(x_0-\xi).$$

On the other hand, since $\psi(x)$ must be continuous everywhere, in the limit $\xi \to 0$, we have

$$\int_{x_0-\xi}^{x_0+\xi} V(x)\,\psi(x)\, dx \simeq \psi(x_0) \int_{x_0-\xi}^{x_0+\xi} V(x)\, dx,$$

and

$$\int_{x_0-\xi}^{x_0+\xi} \psi(x)\, dx \simeq \psi(x_0) \int_{x_0-\xi}^{x_0+\xi} dx = 2\xi\,\psi(x_0).$$

Substituting all this in eq. (1.2) above, we get

$$-\frac{\hbar^2}{2m}\Big[\psi'(x_0+\xi) - \psi'(x_0-\xi)\Big] + \psi(x_0) \int_{x_0-\xi}^{x_0+\xi} V(x)\, dx = \cancelto{0}{2\xi\, E\,\psi(x_0)},$$

where the last term goes to 0 in the limit $\xi \to 0$. Rearranging what remains, we have

$$\psi'(x_0+\xi) - \psi'(x_0-\xi) = \frac{2m\psi(x_0)}{\hbar^2} \int_{x_0-\xi}^{x_0+\xi} V(x)\, dx.$$

If we now take the limit $\xi \to 0$ in the above expression and use the notation

$$\lim_{\xi\to 0} \psi'(x_0+\xi) = \psi'(x_0^+), \qquad \lim_{\xi\to 0} \psi'(x_0-\xi) = \psi'(x_0^-),$$

we finally obtain:

$$\psi'(x_0^+) - \psi'(x_0^-) = \frac{2m\psi(x_0)}{\hbar^2} \lim_{\xi\to 0} \int_{x_0-\xi}^{x_0+\xi} V(x)\, dx. \tag{1.3}$$

This result is completely general and applies for any potential $V(x)$. It tells us whether $\psi'(x)$ is continuous or discontinuous at a given point x_0, depending on the behaviour of the potential there. (See the extended discussion of this in the commented solution to “Problema 5 | Poço de potencial infinito com delta repulsivo” in “Folha de Problemas 9”).

For the specific potential given in the current problem, the point of interest is $x_0 = 0$ (which is the location of the Dirac-delta potential). Putting $x_0 = 0$ and $V(x) = -V_0 a\,\delta(x)$, Eq. (1.3) becomes

$$\psi'(0^+) - \psi'(0^-) = \frac{2m\psi(0)}{\hbar^2} \int_{-\xi}^{+\xi} \big[-V_0 a\,\delta(x)\big]\, dx = -\frac{2mV_0 a\psi(0)}{\hbar^2}. \qquad (\xi \to 0)$$

This last result establishes the condition that the derivative of the wavefunction must obey at the point $x = 0$:

$$\psi'(0^+) - \psi'(0^-) = -\frac{2mV_0 a}{\hbar^2}\,\psi(0). \tag{1.4}$$

2. When $E < 0$ the TISE for this problem reads

$$\psi''(x) = \lambda^2 \psi(x), \qquad \lambda \equiv \sqrt{-\frac{2mE}{\hbar^2}} > 0,$$

which applies everywhere except precisely at the origin. Since we seek a negative energy solution, λ is a real positive number. The general solution of the TISE is then

$$\psi(x) = \begin{cases} Ae^{\lambda x} + Be^{-\lambda x}, & x > 0 \\ Ce^{\lambda x} + De^{-\lambda x}, & x < 0 \end{cases}$$

but a square integrable $\psi(x)$ is only possible if $A = D = 0$. Moreover, since the wavefunction must be continuous at $x = 0$, we need

$$Be^{-\lambda x}\Big|_{x=0} = Ce^{\lambda x}\Big|_{x=0} \qquad \Rightarrow \qquad B = C.$$

Therefore, we can write the solution in the entire space as

$$\psi(x) = B \begin{cases} e^{-\lambda x}, & x > 0 \\ e^{\lambda x}, & x < 0 \end{cases} = Be^{-\lambda |x|}.$$

We can determine B from the normalization condition

$$1 = |B|^2 \int_{-\infty}^{+\infty} e^{-2\lambda |x|} dx = 2\,|B|^2 \int_{0}^{+\infty} e^{-2\lambda x} dx = \frac{|B|^2}{\lambda} \qquad \longrightarrow \qquad B = \sqrt{\lambda},$$

so that the normalized solution is

$$\psi(x) = \sqrt{\lambda}\, e^{-\lambda |x|}. \tag{1.5}$$

We must also ensure the derivative at the origin obeys the relation (1.4) derived in the previous question:

$$\psi'(0^+) - \psi'(0^-) = -\frac{2maV_0}{\hbar^2}\psi(0).$$

Applying this to the wavefunction written in (1.5), we get

$$\sqrt{\lambda}\left(\frac{d}{dx}e^{-\lambda x}\right)_{x=0^+} - \sqrt{\lambda}\left(\frac{d}{dx}e^{\lambda x}\right)_{x=0^-} = -\frac{2maV_0}{\hbar^2}\sqrt{\lambda} \quad \Leftrightarrow \quad \lambda = \frac{maV_0}{\hbar^2}.$$

So, we find that there is indeed one solution with $E < 0$. (It is the only bound solution for this potential because the above equation for λ has no more solutions.) The energy of this bound state is

$$E_0 = -\frac{\hbar^2 \lambda^2}{2m} = -\frac{ma^2 V_0^2}{2\hbar^2}.$$

and the corresponding normalized wavefunction is

$$\varphi_0(x) = \sqrt{\frac{maV_0}{\hbar^2}}\,\exp\left(-\frac{maV_0}{\hbar^2}\,|x|\right).$$

3. By definition, if the wavefunction is normalized, such probability will be

$$\mathcal{P}(-a < x < a) = \int_{-a}^{+a} |\psi(x)|^2\, dx = 2\lambda \int_0^a e^{-2\lambda x} dx = 1 - e^{-2\lambda a} = 1 - \exp\left(-\frac{2ma^2 V_0}{\hbar^2}\right).$$

4. **Short answer:** No, because, if $V_0 < 0$, the potential does not have a minimum anywhere, as can be seen by considering this repulsive Dirac-delta potential as the limit of a rectangular potential barrier. If a potential has no minimum anywhere, there can't be any bound solutions.

   Another answer: Note that, if we make $V_0 < 0$, the potential $V(x)$ becomes repulsive instead of attractive, because the overall prefactor $-V_0 a$ that multiplies the $\delta(x)$ becomes positive [so $V(x)$ becomes a potential barrier if $V_0 < 0$, instead of a potential well when $V_0 > 0$]. Since the potential is zero at $\pm\infty$, any bound states can only exist for $E < 0$. (Bound solutions of the TISE only exist for energies below the smallest of the asymptotic values of the potential at $x = \pm\infty$.) We have considered the general solution for $E < 0$ in question 2 above and saw that it must have the form

$$\psi(x) = \sqrt{\lambda}e^{-\lambda|x|}, \qquad \text{where} \qquad \lambda = \sqrt{-\frac{2mE}{\hbar^2}} > 0, \tag{1.6}$$

   and it must obey the boundary condition

$$\psi'(0^+) - \psi'(0^-) = -\frac{2maV_0}{\hbar^2}\psi(0).$$

   We saw that the combination of these two conditions imply that

$$\lambda = \frac{maV_0}{\hbar^2}.$$

   But, if $V_0 < 0$ this would mean that λ should be negative, which contradicts the definition of λ in eq. (1.6). Thus, (1.6) is not a solution of the TISE for $V_0 < 0$. Since there is no other solution to the combined boundary conditions above, the repulsive Dirac-delta potential has no bound solutions.

5. When $E > 0$, the TISE for this problem reads

$$\psi''(x) = -k^2\psi(x), \qquad k = \sqrt{\frac{2mE}{\hbar^2}} > 0,$$

   everywhere except precisely at the origin. The general solution of the TISE is then (up to a global normalization constant that becomes irrelevant in the case of scattering problems):

$$\psi(x) = \begin{cases} e^{ikx} + r\,e^{-ikx}, & x < 0 \\ t\,e^{ikx} + b\,e^{-ikx}, & x > 0 \end{cases},$$

   where r, t and b are constants to be determined by the boundary conditions. Since we are interested in the scattering problem, we consider that the incoming and reflected waves are on the region $x < 0$ and the transmitted wave propagates in the region $x > 0$. This means that we should put $b = 0$ in the above general solution, because the term $b\,e^{-ikx}$ represents a wave moving from right to left (from $+\infty$ to $-\infty$), which is absent when the particles are launched from $-\infty$ towards the potential (in this situation, only transmitted particles, which move to the right, should be present in the region $x > 0$). This means that, to analyze the scattering problem we begin with the simpler general solution

$$\psi(x) = \begin{cases} e^{ikx} + r\,e^{-ikx}, & x < 0 \\ t\,e^{ikx}, & x > 0 \end{cases}. \tag{1.7}$$

We now have to match $\psi(x)$ and its derivative at $x = 0$ by imposing the boundary conditions we have established in question 1:

$$\psi(0^-) = \psi(0^+) \qquad \text{and} \qquad \psi'(0^+) - \psi'(0^-) = -\frac{2maV_0}{\hbar^2}\psi(0).$$

These two conditions become

$$\begin{cases} 1 + r = t \\ ikt - ik(1-r) = -\frac{2maV_0}{\hbar^2} t \end{cases} \Leftrightarrow \begin{cases} 1 + r = t \\ 1 - r = t\,(1 - 2i\beta) \end{cases} \Leftrightarrow \begin{cases} t = \frac{1}{1-i\beta} \\ r = \frac{i\beta}{1-i\beta} \end{cases} ,$$

where, for convenience, we introduced

$$\beta = \frac{maV_0}{k\hbar^2}, \qquad \text{and note that} \quad \beta^2 = \frac{ma^2V_0^2}{2E\hbar^2}.$$

Finally, we recall that the transmission and reflection coefficients are defined as the ratios of the transmitted and reflected currents to the incoming one:

$$T = \frac{\mathcal{J}_t}{\mathcal{J}_i} = |t|^2 , \qquad R = \frac{\mathcal{J}_r}{\mathcal{J}_i} = |r|^2 . \tag{1.8}$$

To understand what these 3 currents are, we recall that the current density, $\mathcal{J}(x)$, is defined as (see notes for “Lição 18”)

$$\mathcal{J}(x) \equiv \frac{\hbar}{2mi}\left[\psi^*(x)\frac{d}{dx}\psi(x) - \psi(x)\frac{d}{dx}\psi^*(x)\right]. \tag{1.9}$$

To obtain the current density in the region $x > 0$, we replace the wavefunction written in eq. (1.7) in the definition (1.9):

$$\begin{aligned} \mathcal{J}(x>0) &= \frac{\hbar}{2mi}\left[(te^{ikx})^*\frac{d}{dx}(te^{ikx}) - (te^{ikx})\frac{d}{dx}(te^{ikx})^*\right] \\ &= \frac{\hbar}{2mi}\left[(te^{ikx})^*(ikte^{ikx}) - (te^{ikx})(ikte^{ikx})^*\right] \\ &= \frac{\hbar}{2mi}\left[iktt^* + iktt^*\right] = \frac{\hbar k}{m}|t|^2. \end{aligned}$$

Since there is only transmitted probability in the region $x > 0$ (or, equivalently, transmitted particles), such current must correspond to the transmitted current:

$$\mathcal{J}_t = \mathcal{J}(x>0) = \frac{\hbar k}{m}|t|^2.$$

For the region $x < 0$, replacing now the first branch of $\psi(x)$ in eq. (1.7) in the definition (1.9) and proceeding as we did above, you can easily show that

$$\mathcal{J}(x<0) = \underbrace{\frac{\hbar k}{m}}_{\mathcal{J}_i} - \underbrace{\frac{\hbar k}{m}|r|^2}_{\mathcal{J}_r}.$$

In the region $x < 0$ we physically expect to have both incoming particles and particles that have been reflected by the potential. The two terms in the last expression represent precisely the incoming current density (or, equivalently, the flux of incoming particles launched from $-\infty$), $\mathcal{J}_i$, and the reflected current density, $\mathcal{J}_r$:

$$\mathcal{J}_i = \frac{\hbar k}{m}, \qquad \mathcal{J}_r = \frac{\hbar k}{m}|r|^2.$$

Replacing these $\mathcal{J}_{i,r,t}$ in the expressions (1.8) for the transmission and reflection coefficients, we obtain

$$T = \frac{\mathcal{J}_t}{\mathcal{J}_i} = |t|^2 = \frac{1}{1+\beta^2} = \frac{1}{1+\frac{ma^2V_0^2}{2E\hbar^2}}, \qquad R = \frac{\mathcal{J}_r}{\mathcal{J}_i} = |r|^2 = \frac{\beta^2}{1+\beta^2} = \frac{1}{1+\frac{2E\hbar^2}{ma^2V_0^2}}.$$

As a verification that we didn't do any mistake in these calculations, we can always check if

$$T + R \stackrel{?}{=} 1 \qquad \longrightarrow \qquad \frac{\beta^2}{1+\beta^2} + \frac{1}{1+\beta^2} = 1. \quad \checkmark$$

Note: Recall that we must always obtain $R + T = 1$ in any scattering problem because the current density is conserved everywhere. This conservation implies that $\mathcal{J}(x > 0) = \mathcal{J}(x < 0)$ (total current to the left of the potential must equal the total current to the right of the potential) and, if we recall the results above for these two current densities, this means that

$$\mathcal{J}(x > 0) = \mathcal{J}(x < 0) \quad \Leftrightarrow \quad \frac{\hbar k}{m}|t|^2 = \frac{\hbar k}{m} - \frac{\hbar k}{m}|r|^2 \quad \Leftrightarrow \quad \mathcal{J}_t = \mathcal{J}_i - \mathcal{J}_r$$
$$\Downarrow$$
$$T + R = 1.$$

So the statement $R + T = 1$ is equivalent to the statement that the sum of $\mathcal{J}_r$ and $\mathcal{J}_t$ must be equal to the incident current, $\mathcal{J}_i$.

Problema 2 | Oscilador harmónico

Os operadores Hamiltoniano, "destruição" e "número" para o potencial harmónico em 1D são os seguintes:

$$\hat{\mathrm{H}} = \frac{\hat{\mathrm{P}}^2}{2m} + \frac{1}{2}m\omega^2\hat{\mathrm{X}}^2, \qquad a = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{\mathrm{X}} + i\sqrt{\frac{1}{2m\hbar\omega}}\,\hat{\mathrm{P}}, \qquad \hat{\mathrm{N}} = a^\dagger a.$$

Os autoestados de energia $|\varphi_n\rangle$ podem relacionar-se através do operador a de acordo com

$$a|\varphi_n\rangle = \sqrt{n}|\varphi_{n-1}\rangle, \qquad a^\dagger|\varphi_n\rangle = \sqrt{n+1}|\varphi_{n+1}\rangle, \qquad n = 0, 1, 2, \ldots \tag{$\star$}$$

1. Mostre explicitamente que o Hamiltoniano se pode escrever como

$$\hat{\mathrm{H}} = \hbar\omega\Big(a^\dagger a + \frac{1}{2}\Big).$$

2. Recorrendo às propriedades referidas em ($\star$), determine o espectro de energia, E_n.

3. Mostre que, se uma partícula for preparada no estado inicial

$$|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}|\varphi_0\rangle + \frac{1}{\sqrt{2}}|\varphi_1\rangle,$$

o valor esperado da sua posição varia no tempo como

$$\langle\hat{X}\rangle(t) = \sqrt{\frac{\hbar}{2m\omega}}\,\cos(\omega t)\,.$$

4. Usando o operador de destruição, *derive* a equação diferencial a que obedece a função de onda do estado fundamental, $\varphi_0(x) = \langle x|\varphi_0\rangle$. Integre essa equação e obtenha $\varphi_0(x)$.

5. Mostre que, num dado autoestado de energia deste potencial, temos

$$\langle\varphi_n|\hat{\mathrm{K}}|\varphi_n\rangle = \langle\varphi_n|\hat{\mathrm{V}}|\varphi_n\rangle = \frac{E_n}{2}, \qquad \hat{\mathrm{K}} \equiv \frac{\hat{\mathrm{P}}^2}{2m},$$

onde E_n é a energia associada ao autoestado $|\varphi_n\rangle$ e $\hat{\mathrm{K}}$ o operador energia cinética.

6. Na descrição clássica, uma partícula com energia E não poderia visitar as regiões do espaço além dos pontos de viragem, x_M, definidos pela condição $V(x_M) = E$. Se a partícula quântica estiver no estado fundamental, qual é a probabilidade de a encontrar em qualquer ponto da região classicamente proibida?

Nota — Os resultados seguintes poderão ser úteis:

$$\int_{-\infty}^{+\infty} e^{-ax^2}dx = \sqrt{\frac{\pi}{a}}, \quad (\mathrm{Re}\, a > 0)\,, \qquad \int_1^{+\infty} e^{-y^2}dy \simeq 0.14.$$

Solution

1. Looking at the definition of the destruction operator

$$a = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{X} + i\sqrt{\frac{1}{2m\hbar\omega}}\,\hat{P}$$

and inverting this relation for $\hat{X}$ and $\hat{P}$ we have

$$\hat{X} = \sqrt{\frac{\hbar}{2m\omega}}\big(a + a^\dagger\big), \qquad \hat{P} = i\sqrt{\frac{m\hbar\omega}{2}}\big(a^\dagger - a\big).$$

Direct substitution in the Hamiltonian leads to

$$\begin{aligned}
\hat{H} &= \frac{\hat{P}^2}{2m} + \frac{1}{2}m\omega^2\hat{X}^2 \\
&= -\frac{1}{2m}\,\frac{m\hbar\omega}{2}\big(a^\dagger - a\big)^2 + \frac{1}{2}m\omega^2\,\frac{\hbar}{2m\omega}\big(a + a^\dagger\big)^2 \\
&= -\frac{\hbar\omega}{4}\big(a^\dagger - a\big)^2 + \frac{\hbar\omega}{4}\big(a + a^\dagger\big)^2 \\
&= -\frac{\hbar\omega}{4}\big(a^\dagger a^\dagger + aa - a^\dagger a - aa^\dagger\big) + \frac{\hbar\omega}{4}\big(a^\dagger a^\dagger + aa + a^\dagger a + aa^\dagger\big) \\
&= \frac{\hbar\omega}{2}\big(a^\dagger a + aa^\dagger\big) \\
&\Big\downarrow \text{ use the commutator } [a, a^\dagger] = aa^\dagger - a^\dagger a = 1 \text{ to replace } aa^\dagger \\
&= \frac{\hbar\omega}{2}\big(a^\dagger a + a^\dagger a + 1\big) = \hbar\omega\Big(a^\dagger a + \frac{1}{2}\Big) \qquad \boxdot
\end{aligned}$$

2. We have shown in the previous question that

$$\hat{H} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right).$$

According to the properties given in ($\star$), we have

$$\begin{aligned}\hat{H}|\varphi_n\rangle &= \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)|\varphi_n\rangle = \hbar\omega\, a^\dagger a\,|\varphi_n\rangle + \frac{\hbar\omega}{2}\,|\varphi_n\rangle \\ &= \hbar\omega\, a^\dagger\big(\sqrt{n}\,|\varphi_{n-1}\rangle\big) + \frac{\hbar\omega}{2}\,|\varphi_n\rangle = \hbar\omega\,\sqrt{n}\,\big(a^\dagger|\varphi_{n-1}\rangle\big) + \frac{\hbar\omega}{2}\,|\varphi_n\rangle \\ &= \hbar\omega\,\sqrt{n}\,\sqrt{n}\,|\varphi_n\rangle + \frac{\hbar\omega}{2}\,|\varphi_n\rangle = \underbrace{\hbar\omega\left(n+\frac{1}{2}\right)}_{E_n}|\varphi_n\rangle.\end{aligned}$$

This shows that the energy eigenvalues are

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right), \qquad n = 0, 1, 2, \ldots$$

3. Since

$$\hat{H}|\varphi_0\rangle = \overbrace{\frac{\hbar\omega}{2}}^{E_0}\,|\varphi_0\rangle, \qquad \hat{H}|\varphi_1\rangle = \overbrace{\frac{3\hbar\omega}{2}}^{E_1}\,|\varphi_1\rangle,$$

the time-evolved state is

$$|\psi(t)\rangle = \frac{e^{-iE_0t/\hbar}}{\sqrt{2}}|\varphi_0\rangle + \frac{e^{-iE_1t/\hbar}}{\sqrt{2}}|\varphi_1\rangle = \frac{e^{-i\omega t/2}}{\sqrt{2}}|\varphi_0\rangle + \frac{e^{-i3\omega t/2}}{\sqrt{2}}|\varphi_1\rangle,$$

and the desired expectation value corresponds to

$$\begin{aligned}\langle\psi(t)|\hat{X}|\psi(t)\rangle &= \left[\frac{e^{i\omega t/2}}{\sqrt{2}}\langle\varphi_0| + \frac{e^{i3\omega t/2}}{\sqrt{2}}\langle\varphi_1|\right]\ \hat{X}\ \left[\frac{e^{-i\omega t/2}}{\sqrt{2}}|\varphi_0\rangle + \frac{e^{-i3\omega t/2}}{\sqrt{2}}|\varphi_1\rangle\right] \\ &= \frac{1}{2}\langle\varphi_0|\hat{X}|\varphi_0\rangle + \frac{e^{-i\omega t}}{2}\langle\varphi_0|\hat{X}|\varphi_1\rangle + \frac{e^{i\omega t}}{2}\langle\varphi_1|\hat{X}|\varphi_0\rangle + \frac{1}{2}\langle\varphi_1|\hat{X}|\varphi_1\rangle.\end{aligned}$$

We must determine the matrix elements of $\hat{X}$ above between pairs of energy eigenstates. Quite generically, using the fact that $\hat{X} = \sqrt{\frac{\hbar}{2m\omega}}(a+a^\dagger)$, and using the relations between eigenstates in terms of the operators a and $a^\dagger$, we can write such matrix elements as

$$\begin{aligned}\langle\varphi_{n'}|\hat{X}|\varphi_n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left[\langle\varphi_{n'}|a|\varphi_n\rangle + \langle\varphi_{n'}|a^\dagger|\varphi_n\rangle\right] \\ &= \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\langle\varphi_{n'}|\varphi_{n-1}\rangle + \sqrt{n+1}\langle\varphi_{n'}|\varphi_{n+1}\rangle\right] \\ &= \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\,\delta_{n',n-1} + \sqrt{n+1}\,\delta_{n',n+1}\right].\end{aligned}$$

Hence, the expectation value of the position in our problem becomes

$$\begin{aligned}\langle\psi(t)|\hat{X}|\psi(t)\rangle &= \frac{e^{-i\omega t}}{2}\langle\varphi_0|\hat{X}|\varphi_1\rangle + \frac{e^{i\omega t}}{2}\langle\varphi_1|\hat{X}|\varphi_0\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}}\left[\frac{e^{-i\omega t}}{2} + \frac{e^{i\omega t}}{2}\right] \\ &= \sqrt{\frac{\hbar}{2m\omega}}\ \cos(\omega t).\end{aligned}$$

4. Doing exactly as suggested, we have

$$a|\varphi_0\rangle = 0 \quad \Leftrightarrow \quad \left(\sqrt{\frac{m\omega}{2\hbar}}\,\hat{X} + i\sqrt{\frac{1}{2m\hbar\omega}}\,\hat{P}\right)|\varphi_0\rangle = 0$$

When we project this onto the position basis it becomes

$$m\omega\,\langle x|\hat{X}|\varphi_0\rangle + i\,\langle x|\hat{P}|\varphi_0\rangle = 0 \quad \Leftrightarrow \quad \left(\frac{m\omega}{\hbar}x + \frac{d}{dx}\right)\varphi_0(x) = 0,$$

and, therefore, the wavefunction associated with the ground state is the solution of the equation above. Direct integration presents no difficulty:

$$\begin{aligned}
\left(\frac{m\omega}{\hbar}x + \frac{d}{dx}\right)\varphi_0(x) = 0 \quad &\Leftrightarrow \quad \frac{d\varphi_0}{dx} = -\frac{m\omega}{\hbar}x\,\varphi_0(x) \\
\text{(separation of variables)} \quad &\Leftrightarrow \quad \frac{d\varphi_0}{\varphi_0} = -\frac{m\omega}{\hbar}xdx \\
\text{(integrate both sides)} \quad &\Leftrightarrow \quad \log\left|\frac{\varphi_0(x)}{\varphi_0(x_0)}\right| = -\frac{1}{2}\frac{m\omega}{\hbar}\left(x^2 - x_0^2\right) \\
&\Leftrightarrow \quad \varphi_0(x) = Ae^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}.
\end{aligned}$$

The constant A is obtained from the normalization condition

$$1 = \int_{-\infty}^{+\infty} |\varphi_0(x)|^2\,dx = |A|^2\int_{-\infty}^{+\infty} e^{-\frac{m\omega}{\hbar}x^2}dx = |A|^2\sqrt{\frac{\pi\hbar}{m\omega}} \quad \longrightarrow \quad A = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}},$$

where we used the formula provided at the end of the problem text to evaluate the Gaussian integral. The normalized ground state wavefunction is then

$$\varphi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}.$$

5. First, note that the Hamiltonian is the sum of the kinetic and potential energy:

$$\hat{H} = \hat{K} + \hat{V}.$$

Second, if $|\varphi_n\rangle$ is an energy eigenstate with energy E_n, this means that

$$\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle \qquad \longrightarrow \qquad \langle\varphi_n|\hat{H}|\varphi_n\rangle = E_n.$$

But, on the other hand,

$$\langle\varphi_n|\hat{H}|\varphi_n\rangle = \langle\varphi_n|\hat{K}|\varphi_n\rangle + \langle\varphi_n|\hat{V}|\varphi_n\rangle = E_n. \tag{2.1}$$

This means that, if we compute $\langle\varphi_n|\hat{V}|\varphi_n\rangle$, we can directly obtain $\langle\varphi_n|\hat{K}|\varphi_n\rangle$ using the expression above.

To compute $\langle\varphi_n|\hat{V}|\varphi_n\rangle$ we, again, should express $\hat{X}$ in terms of the creation and destruction operators:

$$\begin{aligned}
\langle\varphi_n|\hat{V}|\varphi_n\rangle &= \frac{1}{2}m\omega^2\langle\varphi_n|\hat{X}^2|\varphi_n\rangle = \frac{1}{2}m\omega^2\langle\varphi_n|\left[\sqrt{\frac{\hbar}{2m\omega}}(a+a^\dagger)\right]^2|\varphi_n\rangle \\
&= \frac{\hbar\omega}{4}\langle\varphi_n|\big(a+a^\dagger\big)^2|\varphi_n\rangle = \frac{\hbar\omega}{4}\langle\varphi_n|a^2+aa^\dagger+a^\dagger a+(a^\dagger)^2|\varphi_n\rangle \\
&= \frac{\hbar\omega}{4}\langle\varphi_n|aa^\dagger+aa^\dagger|\varphi_n\rangle \\
&\Big\downarrow \text{ use the commutator } [a,a^\dagger]=aa^\dagger-aa^\dagger=1 \\
&= \frac{\hbar\omega}{4}\langle\varphi_n|2aa^\dagger+1|\varphi_n\rangle = \frac{\hbar\omega}{2}\,\frac{\langle\varphi_n|\hat{H}|\varphi_n\rangle}{\hbar\omega} = \frac{E_n}{2}.
\end{aligned}$$

Recalling now the result (2.1), we find

$$\langle\varphi_n|\hat{K}|\varphi_n\rangle = E_n - \langle\varphi_n|\hat{V}|\varphi_n\rangle = E_n - \frac{E_n}{2} = \frac{E_n}{2}.$$

In conclusion, we found that, for the quantum harmonic oscillator,

$$\langle\varphi_n|\hat{K}|\varphi_n\rangle = \langle\varphi_n|\hat{V}|\varphi_n\rangle = \frac{E_n}{2}.$$

Note: The procedure used here is not the only way to demonstrate the requested result. Alternatively, we could have done it by separately evaluating both $\langle\varphi_n|\hat{V}^2|\varphi_n\rangle = \frac{1}{2}m\omega^2\langle\varphi_n|\hat{X}^2|\varphi_n\rangle$ and $\langle\varphi_n|\hat{K}^2|\varphi_n\rangle = \frac{1}{2m}\langle\varphi_n|\hat{P}^2|\varphi_n\rangle$ in terms of the operators a, $a^\dagger$, and then using the relations $a|\varphi_n\rangle = \sqrt{n}|\varphi_{n-1}\rangle$ and $a^\dagger|\varphi_n\rangle = \sqrt{n+1}|\varphi_{n+1}\rangle$, analogously to how we solved question 4 above.

6. First, we need to determine the classical turning points. If the particle is in the ground-state, its energy is the lowest allowed by the quantization rule for E_n: $E_0 = \hbar\omega/2$. The classical turning points (x_M) for this energy would be

$$V(x_M) = E_0 \quad\Leftrightarrow\quad \frac{1}{2}m\omega^2x_M^2 = \frac{\hbar\omega}{2} \quad\Leftrightarrow\quad x_M = \pm\sqrt{\frac{\hbar}{m\omega}}.$$

The probability of finding the particle outside the classical region is given by

$$\mathcal{P}(|x|>x_M) = \int_{-\infty}^{-x_M}|\varphi_0(x)|^2\,dx + \int_{+x_M}^{+\infty}|\varphi_0(x)|^2\,dx = 2\int_{+x_M}^{+\infty}|\varphi_0(x)|^2\,dx.$$

It is convenient to perform the following change of variable

$$y = x\sqrt{\frac{m\omega}{\hbar}},$$

after which the above integral becomes

$$\mathcal{P} = 2\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\sqrt{\frac{\hbar}{m\omega}}\int_1^{+\infty}e^{-y^2}dy = \frac{2}{\sqrt{\pi}}\int_1^{+\infty}e^{-y^2}dy.$$

Using the value provided in the problem text for this integral, we obtain the numerical value of the requested probability:

$$\mathcal{P}(|x|>x_M) \simeq \frac{2}{\sqrt{\pi}}\times 0.14 \simeq 0.16.$$