2.9

(a)

H in matrix form $H_{\alpha\beta} = \langle\alpha|H|\beta\rangle$ reads

$$H = \delta \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Eigenstates are $|\pm\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|a'\rangle \pm |a''\rangle)$ and eigenvalues are $\pm\delta$, respectively.

(b)

$$|\alpha; t=0\rangle = |a'\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$$

From $|\pm\rangle \to e^{\mp i\frac{\delta}{\hbar}t}|\pm\rangle$ we have

$$\begin{aligned} |\alpha; t\rangle &= \frac{1}{\sqrt{2}}(e^{-i\frac{\delta}{\hbar}t}|+\rangle + e^{i\frac{\delta}{\hbar}t}|-\rangle) \\ &= \frac{1}{\sqrt{2}}[e^{-i\frac{\delta}{\hbar}t}\frac{1}{\sqrt{2}}(|a'\rangle + |a''\rangle) + e^{i\frac{\delta}{\hbar}t}\frac{1}{\sqrt{2}}(|a'\rangle - |a''\rangle)] \\ &= \cos\frac{\delta}{\hbar}t|a'\rangle - i\sin\frac{\delta}{\hbar}t|a''\rangle \end{aligned}$$

(c)

$$P(t) = |\langle a''|\alpha; t\rangle|^2 = |-i\sin\frac{\delta}{\hbar}t|^2 = \sin^2\frac{\delta}{\hbar}t$$

(d)

For a system with 2 (nearly) orthogonal states with same energies, the said Hamiltonian describes hopping between the two states. For example in a H_2^+ molecule, the electron can be bounded near either one of the two atomic cores, giving two states that are nearly orthogonal. The interaction between one core and the electron near the other core can be described as a perturbation of the form given in this problem, and this interaction results in a split in the energy eigenvalues, forming the bounding and anti-bonding molecular orbitals.

2.10

(a)

The Hamiltonian is of the same form as in 2.9, so the eigenkets are $|\pm\rangle = \frac{1}{\sqrt{2}}(|L\rangle \pm |R\rangle)$ with eigenvalues $\pm\Delta$.

(b)

In analogy with 2.9 where $|a'\rangle = |L\rangle$ and $|a''\rangle = |R\rangle$ we have

$$|L\rangle \to= \cos\frac{\Delta}{\hbar}t|L\rangle - i\sin\frac{\Delta}{\hbar}t|R\rangle$$

and

$$|R\rangle \rightarrow= \cos\frac{\Delta}{\hbar}t|R\rangle - i\sin\frac{\Delta}{\hbar}t|L\rangle$$

so we have

$$\begin{aligned}|\alpha;t\rangle &= e^{-i\frac{H}{\hbar}t}|L\rangle\langle L|\alpha\rangle + e^{i\frac{H}{\hbar}t}|R\rangle\langle R|\alpha\rangle \\ &= (\cos\frac{\Delta}{\hbar}t|L\rangle - i\sin\frac{\Delta}{\hbar}t|R\rangle)\langle L|\alpha\rangle + (\cos\frac{\Delta}{\hbar}t|R\rangle - i\sin\frac{\Delta}{\hbar}t|L\rangle)\langle R|\alpha\rangle \\ &= \cos\frac{\Delta}{\hbar}t|\alpha\rangle - i\sin\frac{\Delta}{\hbar}t(|R\rangle\langle L|\alpha\rangle + |L\rangle\langle R|\alpha\rangle)\end{aligned}$$

(c)

For $|\alpha\rangle = |R\rangle$, $\langle L|\alpha\rangle = 0$ and $\langle R|\alpha\rangle = 1$, then $|\alpha;t\rangle = \cos\frac{\Delta}{\hbar}t|R\rangle - i\sin\frac{\Delta}{\hbar}t|L\rangle$. So we have

$$P(t) = |\langle L|\alpha;t\rangle|^2 = |-i\sin\frac{\Delta}{\hbar}t|^2 = \sin^2\frac{\Delta}{\hbar}t$$

(d)

The coupled Schrödinger equations read

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\langle L|\alpha;t\rangle \\ \langle R|\alpha;t\rangle\end{pmatrix} = \Delta\begin{pmatrix}0 & 1 \\ 1 & 0\end{pmatrix}\begin{pmatrix}\langle L|\alpha;t\rangle \\ \langle R|\alpha;t\rangle\end{pmatrix}$$

and the solutions are

$$\begin{aligned}\langle L|\alpha;t\rangle &= \cos\frac{\Delta}{\hbar}t\langle L|\alpha\rangle - i\sin\frac{\Delta}{\hbar}t\langle R|\alpha\rangle \\ \langle R|\alpha;t\rangle &= -i\sin\frac{\Delta}{\hbar}t\langle L|\alpha\rangle + \cos\frac{\Delta}{\hbar}t\langle R|\alpha\rangle\end{aligned}$$

and are the same as in (b).

(e)

The equations now read

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\langle L|\alpha;t\rangle \\ \langle R|\alpha;t\rangle\end{pmatrix} = \Delta\begin{pmatrix}0 & 1 \\ 0 & 0\end{pmatrix}\begin{pmatrix}\langle L|\alpha;t\rangle \\ \langle R|\alpha;t\rangle\end{pmatrix}$$

and the solutions are

$$\begin{aligned}\langle L|\alpha;t\rangle &= \langle L|\alpha\rangle - i\frac{\Delta}{\hbar}t\langle R|\alpha\rangle \\ \langle R|\alpha;t\rangle &= \langle R|\alpha\rangle\end{aligned}$$

Now for $|\alpha;t>0\rangle$ we have

$$\langle\alpha;t|\alpha;t\rangle = |\langle L|\alpha\rangle|^2 + (1+\frac{\Delta^2}{\hbar^2}t^2)|\langle R|\alpha\rangle|^2$$

If $|\alpha\rangle$ is normalized, that is, $|\langle L|\alpha\rangle|^2 + |\langle R|\alpha\rangle|^2 = 1$, then it's clear that $\langle\alpha;t|\alpha;t\rangle > 1$ for $t > 0$, so that probability is not conserved.

2.12

In Heisenberg picture there is

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{1}{i\hbar}[x, H] = \frac{p}{m}$$
$$\frac{\mathrm{d}p}{\mathrm{d}t} = \frac{1}{i\hbar}[p, H] = -m\omega^2 x$$

using results from 1.29. The solution is

$$x = x_0 \mathrm{cos}\omega t + \frac{p_0}{m\omega}\mathrm{sin}\omega t$$
$$p = -x_0 m\omega \mathrm{sin}\omega t + p_0 \mathrm{cos}\omega t$$

where x_0 and p_0 are operators at time $t = 0$. For the given state, we have

$$\langle 0|e^{\frac{ip_0 a}{\hbar}} p_0 e^{\frac{-ip_0 a}{\hbar}}|0\rangle = \langle 0|p_0 e^{\frac{ip_0 a}{\hbar}} e^{\frac{-ip_0 a}{\hbar}}|0\rangle = \langle 0|p_0|0\rangle = 0$$

and because $e^{\frac{-ip_0 a}{\hbar}}$ is the translation operator $\mathscr{J}(a)$, we have

$$\langle 0|e^{\frac{ip_0 a}{\hbar}} x_0 e^{\frac{-ip_0 a}{\hbar}}|0\rangle = \langle 0|x_0|0\rangle + a = a$$

thus

$$\langle 0|e^{\frac{ip_0 a}{\hbar}} x e^{\frac{-ip_0 a}{\hbar}}|0\rangle = \langle 0|e^{\frac{ip_0 a}{\hbar}} x_0 e^{\frac{-ip_0 a}{\hbar}}|0\rangle \mathrm{cos}\omega t + \frac{\langle 0|e^{\frac{ip_0 a}{\hbar}} p_0 e^{\frac{-ip_0 a}{\hbar}}|0\rangle}{m\omega}\mathrm{sin}\omega t = a\mathrm{cos}\omega t$$

which is similar to the classic result.

2.14

(a)

From the definition of a and $a^\dagger$, we have

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \quad p = \frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}(a - a^\dagger)$$

so that

$$
\begin{aligned}
\langle m|x|n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}(\langle m|\sqrt{n}|n-1\rangle + \langle m|\sqrt{n+1}|n+1\rangle) \\
&= \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}) \\
\langle m|p|n\rangle &= \frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}(\langle m|\sqrt{n}|n-1\rangle - \langle m|\sqrt{n+1}|n+1\rangle) \\
&= \frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}(\sqrt{n}\delta_{m,n-1} - \sqrt{n+1}\delta_{m,n+1}) \\
\langle m|\{x,p\}|n\rangle &= \frac{\hbar}{i}\langle m|(aa - a^\dagger a^\dagger)|n\rangle \\
&= \frac{\hbar}{i}(\langle m|\sqrt{n(n-1)}|n-2\rangle - \langle m|\sqrt{(n+1)(n+2)}|n+2\rangle) \\
&= \frac{\hbar}{i}(\sqrt{n(n-1)}\delta_{m,n-2} - \sqrt{(n+1)(n+2)}\delta_{m,n+2}) \\
\langle m|x^2|n\rangle &= \frac{\hbar}{2m\omega}\langle m|(aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)|n\rangle \\
&= \frac{\hbar}{2m\omega}(\sqrt{n(n-1)}\delta_{m,n-2} + (2n+1)\delta_{m,n} + \sqrt{(n+1)(n+2)}\delta_{m,n+2}) \\
\langle m|p^2|n\rangle &= -\frac{m\hbar\omega}{2}\langle m|(aa - aa^\dagger - a^\dagger a + a^\dagger a^\dagger)|n\rangle \\
&= -\frac{m\hbar\omega}{2}(\sqrt{n(n-1)}\delta_{m,n-2} - (2n+1)\delta_{m,n} + \sqrt{(n+1)(n+2)}\delta_{m,n+2})
\end{aligned}
$$

(b)

For $m = n$, we have

$$
\begin{aligned}
\langle T\rangle &= \frac{\langle n|p^2|n\rangle}{2m} = \frac{1}{2m}\frac{m\hbar\omega(2n+1)}{2} = \frac{(2n+1)\hbar\omega}{4} \\
\langle V\rangle &= \frac{m\omega^2\langle n|x^2|n\rangle}{2} = \frac{m\omega^2}{2}\frac{\hbar(2n+1)}{2m\omega} = \frac{(2n+1)\hbar\omega}{4}
\end{aligned}
$$

so that $\langle T\rangle = \langle V\rangle$ in accordance with the Virial theorem.

2.22

(a)

The Hamiltonian, thus the Schrödinger equation, in region $x > 0$ is identical to that of a harmonic oscillator, so the wave function in region $x > 0$ should be identical as well. In region $x < 0$ the wave function should be zero, which requires $\psi(0) = 0$. We can see that the functions

$$
\psi_n(x) = \begin{cases} \sqrt{2}\langle x|2n+1\rangle & x \geq 0 \\ 0 & x < 0 \end{cases} \quad n = 0, 1, 2, \cdots
$$

is a set of orthonormal functions satisfying said restrictions, where $|2n+1\rangle$ is the $(2n+1)$ th eigenstate of the harmonic oscillator with potential $V = \frac{1}{2}kx^2$. Furthermore, this set of functions is complete, following from the completeness of the eigenkets of harmonic oscillators, and by checking we can conclude that $\psi_n(x)$ is the nth eigenstate of the given system with energy eigenvalue $E_n = (2n+1+\frac{1}{2})\hbar\omega$. So the ground-state energy is $E_0 = \frac{3}{2}\hbar\omega = \frac{3}{2}\hbar\sqrt{\frac{k}{m}}$.

(b)

$$\langle x^2\rangle = \int_0^{+\infty}\psi_0^*(x)x^2\psi_0(x)\mathrm{d}x = 2\int_0^{+\infty}\langle 1|x\rangle x^2\langle x|1\rangle\mathrm{d}x = \int_{-\infty}^{+\infty}\langle 1|x\rangle x^2\langle x|1\rangle\mathrm{d}x = \langle 1|x^2|1\rangle$$

From 2.14 we have $\langle x^2\rangle = \frac{3\hbar}{2m\omega}$.

2.23

The wave function at $t=0$ is $\psi(x)=\delta(x-L/2)$. So we have

$$\langle\alpha|n\rangle = \int_0^L \mathrm{d}x\delta(x-L/2)\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} = \sqrt{\frac{2}{L}}\sin\frac{n\pi}{2}$$

$$|\langle\alpha|n\rangle|^2 = \begin{cases}\dfrac{2}{L} & n=2k-1 \\ 0 & n=2k\end{cases} \qquad k=1,2,3,\cdots$$

So the probability of finding the particle in eigenstates $|2k-1\rangle$ are all the same, while for $|2k\rangle$ the probabilities are zero. Since we can write

$$|\alpha\rangle = \sum_n |n\rangle\langle n|\alpha\rangle = \sqrt{\frac{2}{L}}\sum_{n=1}^{+\infty}|2n-1\rangle(-1)^{n-1}$$

we have

$$\begin{aligned}\psi(x;t) = \langle x|\alpha;t\rangle &= \langle x|\sqrt{\frac{2}{L}}\sum_{n=1}^{+\infty}\exp\left\{-i\frac{1}{\hbar}\frac{\hbar^2}{2m}\left[\frac{(2n-1)\pi}{L}\right]^2 t\right\}|2n-1\rangle(-1)^{n-1} \\ &= \sqrt{\frac{2}{L}}\sum_{n=1}^{+\infty}\exp\left\{-\frac{i\hbar t}{2m}\left[\frac{(2n-1)\pi}{L}\right]^2\right\}\sqrt{\frac{2}{L}}\sin\frac{(2n-1)\pi x}{L}(-1)^{n-1} \\ &= \frac{2}{L}\sum_{n=1}^{+\infty}\exp\left\{-\frac{i\hbar t}{2m}\left[\frac{(2n-1)\pi}{L}\right]^2\right\}\sin\frac{(2n-1)\pi x}{L}(-1)^{n-1}\end{aligned}$$