Appendix 3

Quantum Harmonic Oscillator
(量子谐振子)

Objectives

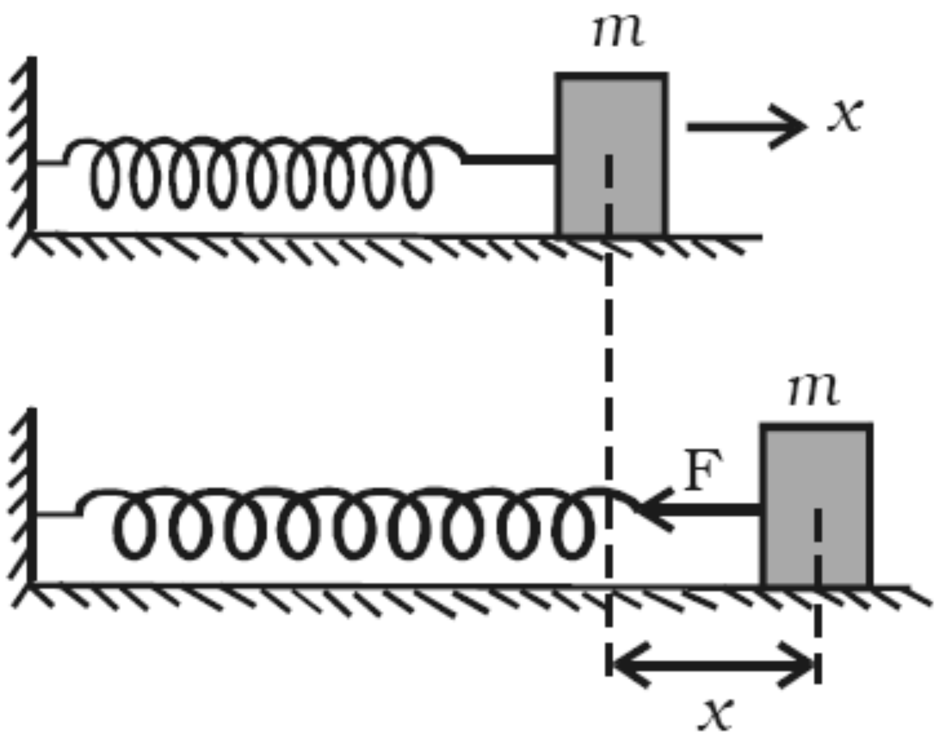
- To learn the **quantum description** of harmonic oscillator.
- To understand the properties of **quantum harmonic oscillator**.

Appendix 3: Quantum Harmonic Oscillator (量子谐振子)

➢ Simple Harmonic Oscillator (简谐振子)

❖ Hook's law (胡克定律):

$$\boldsymbol{F} = -\boldsymbol{K}\boldsymbol{x}$$



Appendix 3: Quantum Harmonic Oscillator (量子谐振子)

➢ Description of Classical Mechanics (经典力学描述)

❖ Equation of motion:

$$\boldsymbol{m\frac{d^2x}{dt^2} = F = -Kx}$$

$$\longrightarrow \quad \boldsymbol{\frac{d^2x}{dt^2} + \omega^2 x = 0} \qquad \boldsymbol{\omega \equiv \sqrt{K/m}}$$

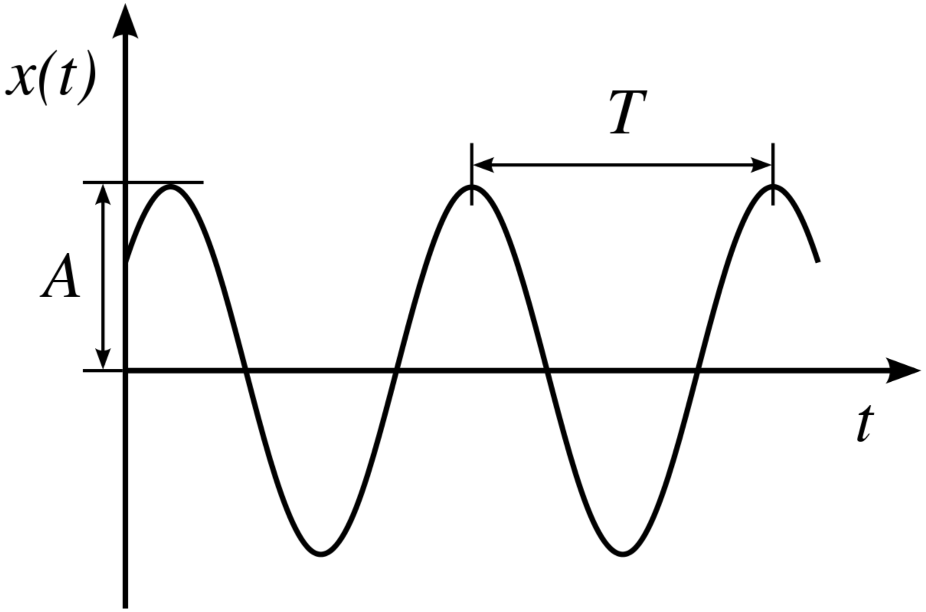
Appendix 3: Quantum Harmonic Oscillator (量子谐振子)

➢ Description of Classical Mechanics (经典力学描述)

❖ Solution:

$$\boldsymbol{x} = \boldsymbol{A}\boldsymbol{e}^{\boldsymbol{i}(\boldsymbol{\omega t}+\boldsymbol{\varphi})}$$

$$\Rightarrow \quad \mathbf{Re}(\boldsymbol{x}) = \boldsymbol{A}\cos(\boldsymbol{\omega t} + \boldsymbol{\varphi})$$



Appendix 3: Quantum Harmonic Oscillator (量子谐振子)

➢ Description of Quantum Mechanics (量子力学描述)

❖ Kinetic energy:

$$T = \frac{1}{2m}p^2 \longrightarrow \hat{T} = \frac{1}{2m}\hat{p}^2$$

❖ Potential energy:

$$V = \frac{1}{2}Kx^2 \longrightarrow \hat{V} = \frac{1}{2}m\omega^2\hat{x}^2$$

❖ Hamiltonian:

$$\hat{H} = \hat{T} + \hat{V} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2$$

Appendix 3: Quantum Harmonic Oscillator (量子谐振子)

➢ **Description of Quantum Mechanics (量子力学描述)**

❖ **The stationary Schrodinger equation (定态薛定谔方程):**

$$\hat{H}\psi = E\psi$$

$$\longrightarrow \quad E\,? \qquad \psi\,?$$

Algebraic Method (代数解法)

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➢ Algebraic Method (代数解法)

❖ For the Hamiltonian $\widehat{H}=\frac{1}{2m}\widehat{p}^2+\frac{1}{2}m\omega^2\widehat{x}^2$, we can define a new pair of operators:

$$\widehat{a}=\sqrt{\frac{m\omega}{2\hbar}}\left(\widehat{x}+\frac{i}{m\omega}\widehat{p}\right) \qquad \widehat{a}^{+}=\sqrt{\frac{m\omega}{2\hbar}}\left(\widehat{x}-\frac{i}{m\omega}\widehat{p}\right)$$

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

Note that $\widehat{a}^{+}$ and $\widehat{a}$ are not Hermitian!

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➢ Algebraic Method (代数解法)

❖ By applying the new forms of $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{p}}$ to the Hamiltonian $\hat{\boldsymbol{H}}$, we can obtain:

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

Note that a commuting relation $[\hat{\boldsymbol{a}}, \hat{\boldsymbol{a}}^{+}] = 1$ is used.

❖ Then, the Schrödinger equation reads:

$$\hbar\boldsymbol{\omega}\left(\hat{\boldsymbol{a}}^{+}\hat{\boldsymbol{a}} + \frac{\mathbf{1}}{\mathbf{2}}\right)\boldsymbol{\psi} = \boldsymbol{E}\boldsymbol{\psi}$$

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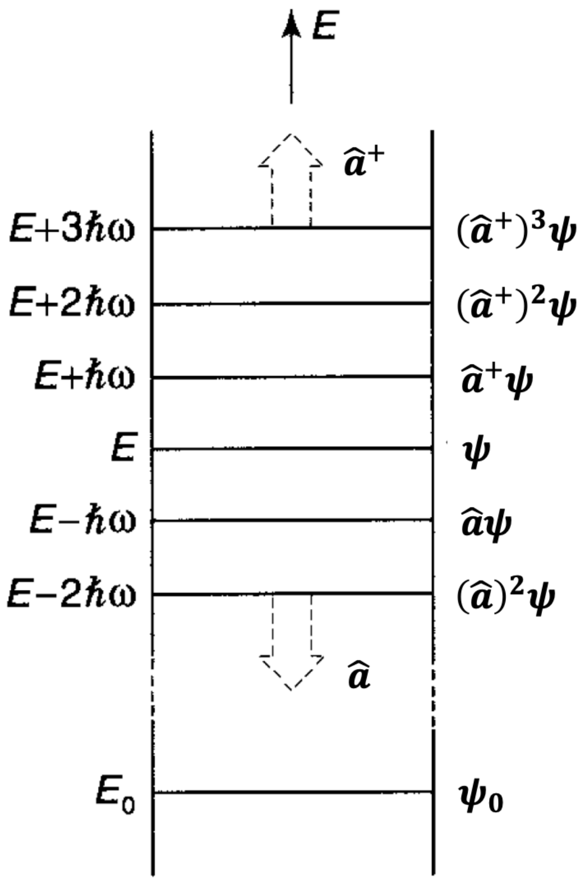
➢ Algebraic Method (代数解法)

❖ Properties of operators $\hat{a}^+$ and $\hat{a}$:

If ψ satisfies the Schrödinger equation with eigenvalue E,

- $\hat{a}^+\psi$ satisfies the Schrödinger equation with eigenvalue $E + \hbar\omega$;
- $\hat{a}\psi$ satisfies the Schrödinger equation with eigenvalue $E - \hbar\omega$;



As a result, $\hat{a}^+$ and $\hat{a}$ are also called **ladder operators (阶梯算符)!**

$\hat{a}^+$ is called the **raising operator** (升算符);

$\hat{a}$ is called the **lowering operator** (降算符).

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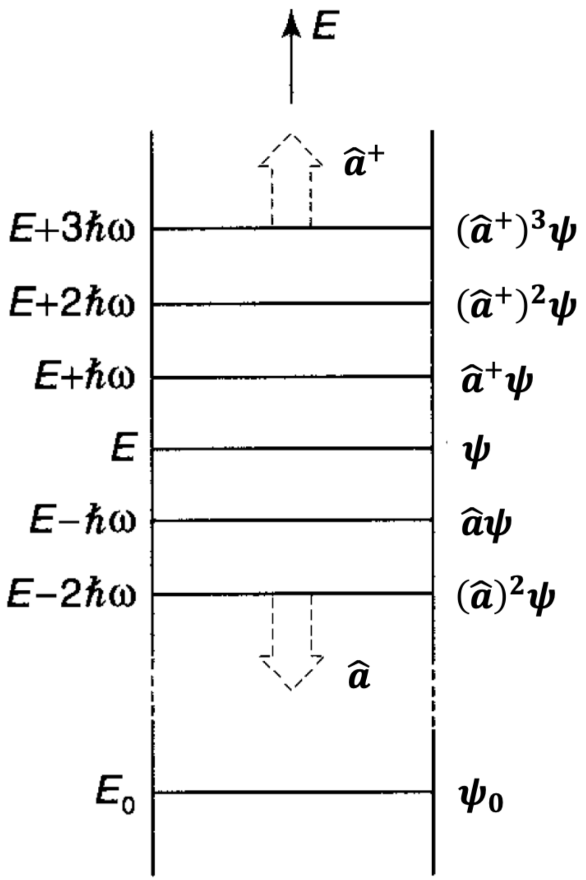
➢ Algebraic Method (代数解法)

❖ The **ground state** (基态) ψ_0 of the harmonic oscillator:

- If $\hat{a}$ is repeatedly applied to ψ, it would end up with a state with energy less than zero, which is meaningless.

- Thus, the lowest possible state ψ_0 (i.e., the **ground state**) of the harmonic oscillator must satisfy:

$$\hat{a}\psi_0 = 0$$



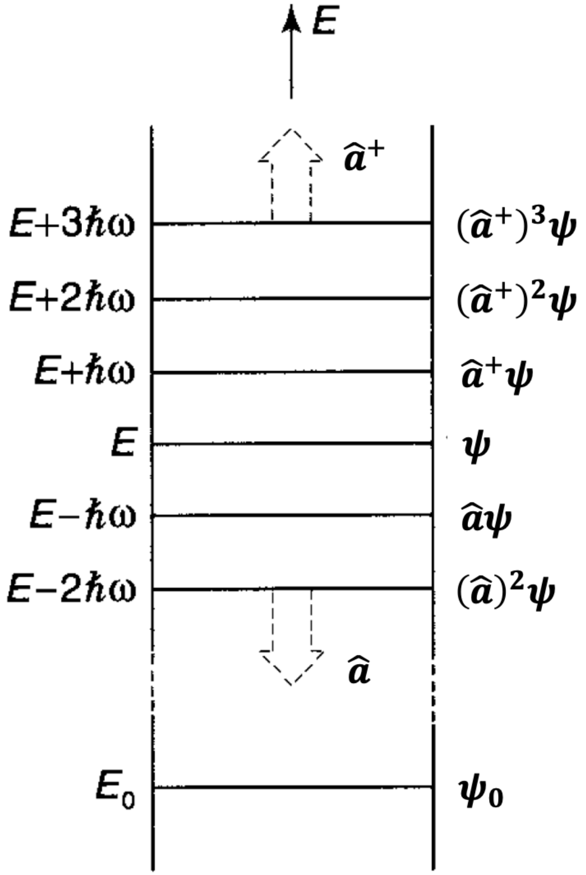
➢ Algebraic Method (代数解法)

❖ The **ground state** (基态) ψ_0 of the harmonic oscillator:

$$\hat{a}\psi_0 = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)\psi_0 = 0$$

$$\hat{p} = -i\hbar\frac{\partial}{\partial x} \quad \longrightarrow \quad \frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar}x\psi_0$$

$$\psi_0(x) = A_0 e^{-\frac{m\omega}{2\hbar}x^2} \qquad E_0 = \frac{1}{2}\hbar\omega$$



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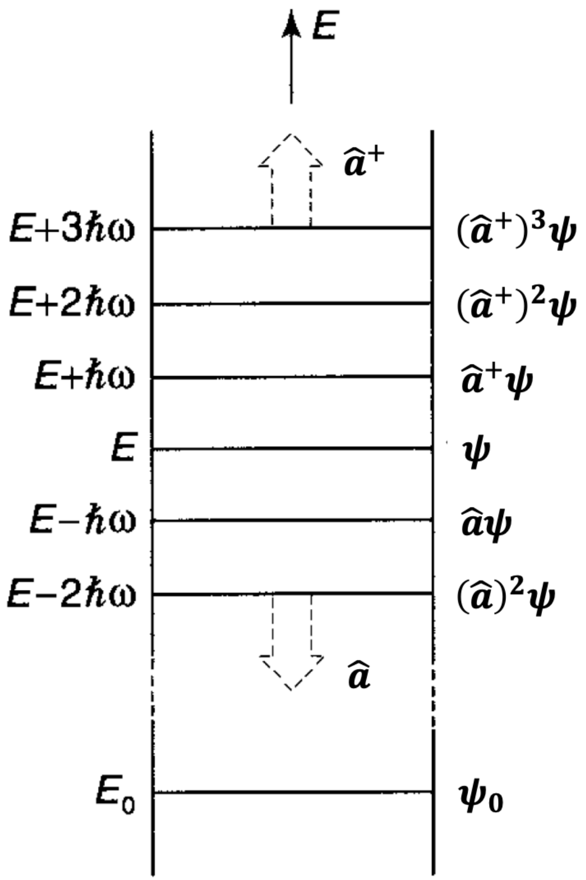
➢ Algebraic Method (代数解法)

❖ The **excited states** (激发态) ψ_n of the harmonic oscillator:

- All the states higher in energy than the ground state, i.e., the **excited states**, can be obtained by repeatedly applying $\hat{a}^+$ to ψ_0:

$$\psi_n(x) = A_n(\hat{a}^+)^n \mathrm{e}^{-\frac{m\omega}{2\hbar}x^2}$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, 3, \cdots$$



Appendix 3: Quantum Harmonic Oscillator (量子谐振子)

➢ Algebraic Method (代数解法)

❖ If we define a number operator $\hat{N} = \hat{a}^{+}\hat{a}$ and let $\psi_n = |n\rangle$, it can be obtained that:

$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$$

$$\hat{N}|n\rangle = n|n\rangle$$

$$\hat{a}^{+}|n\rangle = \sqrt{n+1}|n+1\rangle \qquad \hat{a}|n\rangle = \sqrt{n}|n-1\rangle$$

$$|n\rangle = \frac{(\hat{a}^{+})^{n}}{\sqrt{n!}}|0\rangle$$

Analytic Method (解析解法)

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➢ Analytic Method (解析解法)

❖ In the **position representation** (位置表象), the Schrödinger equation reads:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi$$

By introducing two dimensionless variables:

$$\xi=\sqrt{\frac{m\omega}{\hbar}}x \qquad \varepsilon=\frac{2E}{\hbar\omega}$$

$$\longrightarrow \quad \boxed{\frac{d^2\psi}{d\xi^2}=(\xi^2-\varepsilon)\psi}$$

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➢ Analytic Method (解析解法)

❖ Given the fact that $\boldsymbol{\psi} \to \mathbf{0}$ when $\boldsymbol{x} \to \pm\infty$, by applying some complicated mathematical techniques (omitted here), the **normalized stationary states (归一化定态)** and the corresponding **eigenvalues** of the harmonic oscillator are:

$$\boldsymbol{\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) \mathrm{e}^{-\xi^2/2}}$$

$$\boldsymbol{E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, 3, \cdots}$$

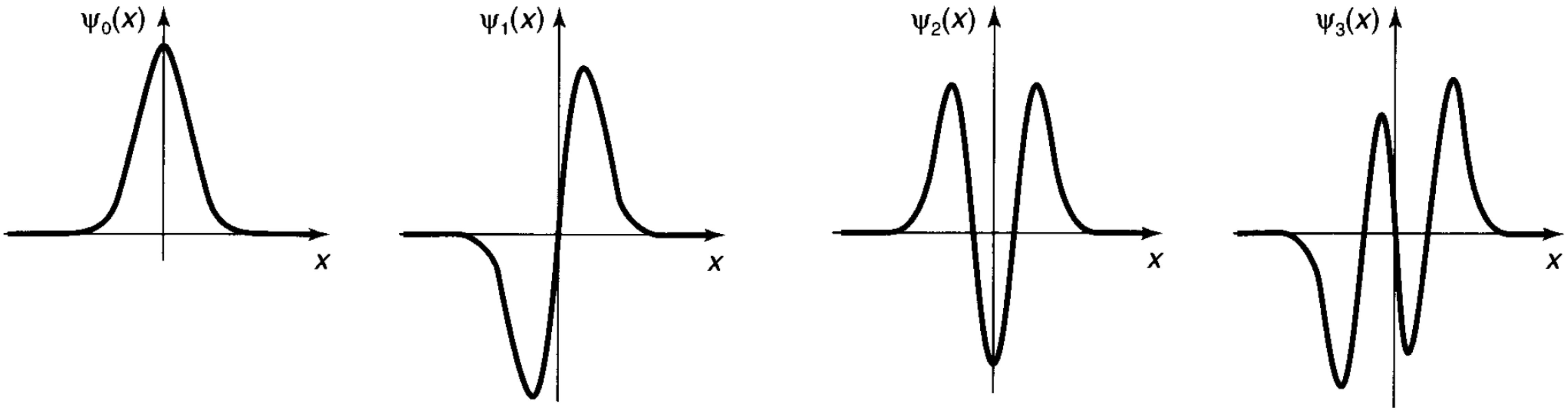
Here, $\boldsymbol{H_n(\xi)}$ denotes the so-called **Hermite polynomials** (厄米多项式), e.g.,

$$H_0(\xi) = 1 \qquad H_1(\xi) = 2\xi \qquad H_2(\xi) = 4\xi^2 - 2 \qquad H_3(\xi) = 8\xi^3 - 12\xi \qquad \cdots$$

Appendix 3: Quantum Harmonic Oscillator (量子谐振子)

- **Analytic Method (解析解法)**

  ❖ The spatial distribution of the wave functions:



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➢ Analytic Method (解析解法)

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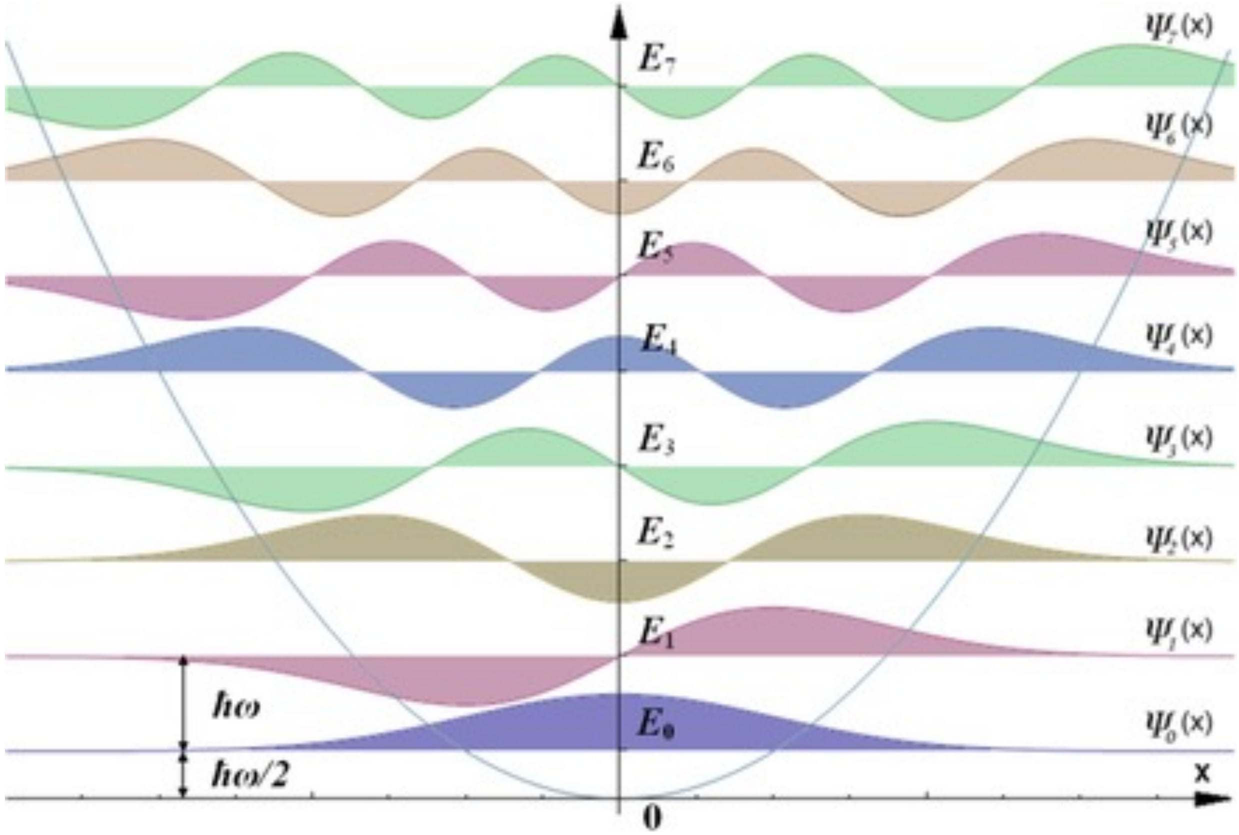

➢ Analytic Method (解析解法)

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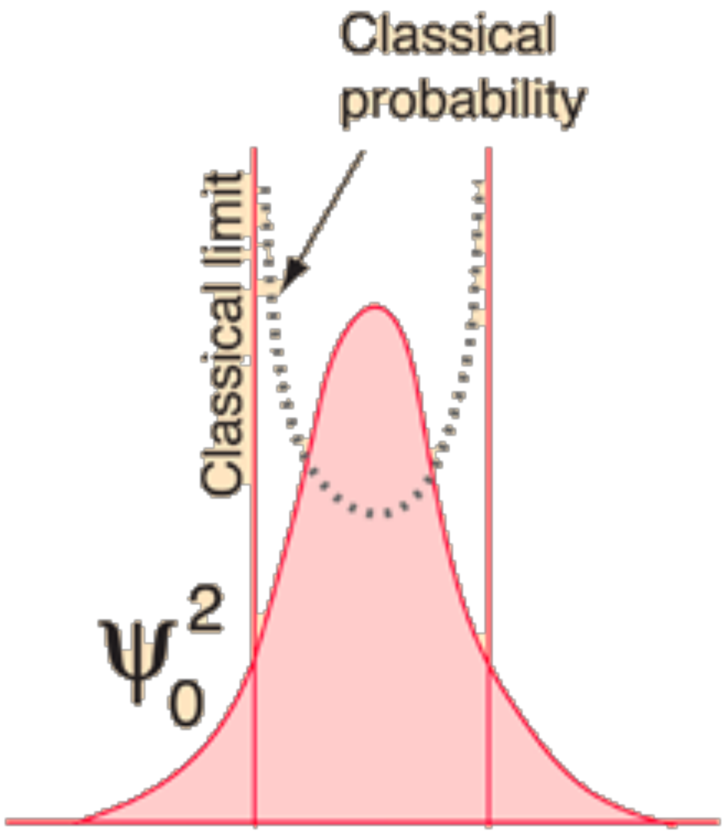

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➢ Analytic Method (解析解法)

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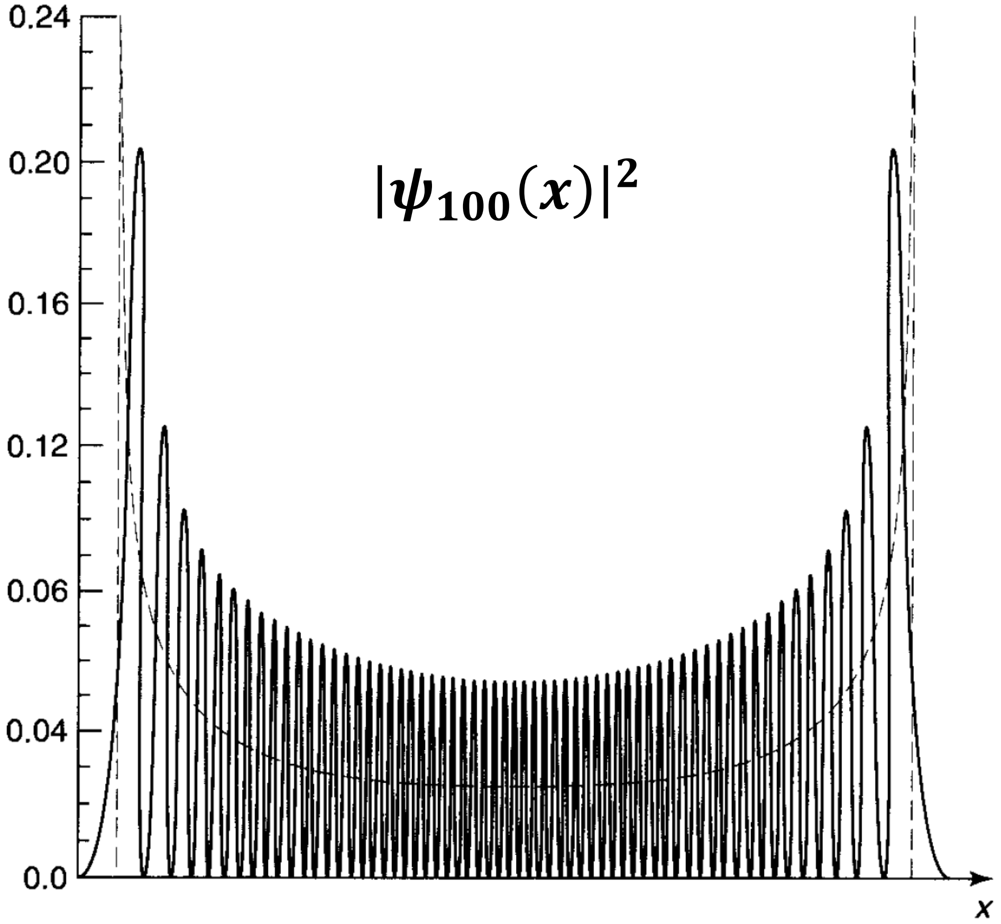

Appendix 3: Quantum Harmonic Oscillator (量子谐振子)

Summary (总结)

Appendix 3: Quantum Harmonic Oscillator (量子谐振子)

➢ Summary (总结)

- The quantum description of harmonic oscillator.

$$\hat{H}\psi = E\psi \qquad \hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2$$

$$\boldsymbol{E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, 3, \cdots}$$

- Algebraic method: **ladder operators**

- Analytic method: **wave functions**