



1.8. Schrodinger Equation $i\hbar \frac{\partial w}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 w}{\partial x^2} + U(x)w$

1.8-1. Eigenvalue problem. Cauchy problem for the Schrodinger's equation.

The Schrodinger's (Schrödinger's) equation is the basic equation of quantum mechanics; w is the wave function, $i^2 = -1$, \hbar is Planck's constant, m is the mass of the particle, and $U(x)$ is the potential energy of the particle in the force field.

1°. In discrete spectrum problems, the particular solutions are sought in the form

$$w(x, t) = \exp\left(-\frac{iE_n t}{\hbar}\right) \psi_n(x),$$

where the eigenfunctions ψ_n and the respective energies E_n have to be determined by solving the eigenvalue problem

$$\begin{aligned} \frac{d^2 \psi_n}{dx^2} + \frac{2m}{\hbar^2} [E_n - U(x)] \psi_n &= 0, \\ \psi_n \rightarrow 0 \text{ at } x \rightarrow \pm\infty, \quad \int_{-\infty}^{\infty} |\psi_n|^2 dx &= 1. \end{aligned} \tag{1}$$

The last relation is the normalizing condition for ψ_n .

2°. In the cases where the eigenfunctions $\psi_n(x)$ form an orthonormal basis in $L_2(\mathbb{R})$, the solution of the Cauchy problem for Schrodinger's equation with the initial condition

$$w = f(x) \quad \text{at} \quad t = 0 \tag{2}$$

is given by

$$w(x, t) = \int_{-\infty}^{\infty} G(x, \xi, t) f(\xi) d\xi, \quad G(x, \xi, t) = \sum_{n=0}^{\infty} \psi_n(x) \psi_n(\xi) \exp\left(-\frac{iE_n t}{\hbar}\right).$$

Various potentials $U(x)$ are considered below and particular solutions of the boundary value problem (1) or the Cauchy problem for Schrodinger's equation are presented.

1.8-2. Free particle: $U(x) = 0$.

The solution of the Cauchy problem for the Schrodinger's equation with the initial condition (2) is given by

$$w(x, t) = \frac{1}{2\sqrt{i\pi\tau}} \int_{-\infty}^{\infty} \exp\left[-\frac{(x-\xi)^2}{4i\tau}\right] f(\xi) d\xi, \quad \tau = \frac{\hbar t}{2m}, \quad \sqrt{ia} = \begin{cases} e^{\pi i/4} \sqrt{|a|} & \text{if } a > 0, \\ e^{-\pi i/4} \sqrt{|a|} & \text{if } a < 0. \end{cases}$$

1.8-3. Linear potential (motion in a uniform external field): $U(x) = ax$.

Solution of the Cauchy problem for the Schrodinger's equation with the initial condition (2):

$$w(x, t) = \frac{1}{2\sqrt{i\pi\tau}} \exp(-ib\tau x - \frac{1}{3}ib^2\tau^3) \int_{-\infty}^{\infty} \exp\left[-\frac{(x+b\tau^2-\xi)^2}{4i\tau}\right] f(\xi) d\xi, \quad \tau = \frac{\hbar t}{2m}, \quad b = \frac{2am}{\hbar^2}.$$

1.8-4. Linear harmonic oscillator: $U(x) = \frac{1}{2}m\omega^2x^2$.

Eigenvalues:

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

Normalized eigenfunctions:

$$\psi_n(x) = \frac{1}{\pi^{1/4}\sqrt{2^n n!}x_0} \exp\left(-\frac{1}{2}\xi^2\right) H_n(\xi), \quad \xi = \frac{x}{x_0}, \quad x_0 = \sqrt{\frac{\hbar}{m\omega}},$$

where $H_n(\xi)$ are the Hermite polynomials. The functions $\psi_n(x)$ form an orthonormal basis in $L_2(\mathbb{R})$.

1.8-5. Isotropic free particle: $U(x) = a/x^2$.

Here, the variable $x \geq 0$ plays the role of the radial coordinate, and $a > 0$. The equation with $U(x) = a/x^2$ results from Schrodinger's equation for a free particle with n space coordinates if one passes to spherical (cylindrical) coordinates and separates the angular variables.

The solution of Schrodinger's equation satisfying the initial condition (2) has the form

$$w(x, t) = \frac{\exp\left[-\frac{1}{2}i\pi(\mu + 1) \operatorname{sign} t\right]}{2|\tau|} \int_0^\infty \sqrt{xy} \exp\left(i\frac{x^2 + y^2}{4\tau}\right) J_\mu\left(\frac{xy}{2|\tau|}\right) f(y) dy,$$

$$\tau = \frac{\hbar t}{2m}, \quad \mu = \sqrt{\frac{2am}{\hbar^2} + \frac{1}{4}} \geq 1,$$

where $J_\mu(\xi)$ is the Bessel function.

1.8-6. Morse potential: $U(x) = U_0(e^{-2x/a} - 2e^{-x/a})$.

Eigenvalues:

$$E_n = -U_0 \left[1 - \frac{1}{\beta} \left(n + \frac{1}{2}\right)\right]^2, \quad \beta = \frac{a\sqrt{2mU_0}}{\hbar}, \quad 0 \leq n < \beta - 2.$$

Eigenfunctions:

$$\psi_n(x) = \xi^s e^{-\xi/2} \Phi(-n, 2s + 1, \xi), \quad \xi = 2\beta e^{-x/a}, \quad s = \frac{a\sqrt{-2mE_n}}{\hbar},$$

where $\Phi(a, b, \xi)$ is the degenerate hypergeometric function.

In this case the number of eigenvalues (energy levels) E_n and eigenfunctions ψ_n is finite: $n = 0, 1, \dots, n_{\max}$.

References

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