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

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

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

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

$$\frac{d^2\psi_n}{dx^2}+\frac{2m}{\hbar^2}\big[E_n-U(x)\big]\psi_n=0,$$
$$\psi_n\to 0 \text{ at } x\to\pm\infty, \qquad \int_{-\infty}^{\infty}|\psi_n|^2\,dx=1. \tag{1}$$

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

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

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

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

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):

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

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

Eigenvalues:

$$E_n = \hbar\omega\bigl(n + \tfrac{1}{2}\bigr), \qquad n = 0,\ 1,\ \ldots$$

Normalized eigenfunctions:

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

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 $x \ge 0$ 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

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

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

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

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

Eigenvalues:

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

Eigenfunctions:

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

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: $n = 0,\ 1,\ \ldots,\ n_{\max}$.

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