21. Time-dependent Schrödinger equation — *probability waves and tunneling*

The Schrödinger equation, the basis of quantum mechanics, was discovered by Erwin Schrödinger during his skiing holiday at the end of 1925 and analyzed by him in a series of papers published in *Annalen der Physik* in 1926. By the end of that year, the face of physics had changed. Schrödinger won the Nobel Prize in Physics in 1933.

For a system of N particles in three dimensions, the Schrödinger equation applies in a state space of dimension $3N$. However, let us consider the familiar case of a single point particle, so that the state space is $\mathbb{R}^3$. Suppose the particle has mass m and is subject to a force $F(\mathbf{r}) = -\nabla V(\mathbf{r})$, where $V(\mathbf{r})$ is a fixed *potential function*. For example, the particle might be an electron attracted to a proton at $\mathbf{r} = 0$ by an inverse square force with $V(\mathbf{r}) = -C/|\mathbf{r}|$ (the hydrogen atom). A physicist would write the equation as

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[-\frac{\hbar}{2m}\Delta + V(\mathbf{r})\right]\Psi(\mathbf{r},t) \qquad (1)$$

where $\mathrm{i} = \sqrt{-1}$, Ψ is called the *wave function* and $\hbar$ is Planck's constant divided by 2π. Since our convention in this book is to take u as the dependent variable and strip away constants, we shall take the *time-dependent Schrödinger equation* instead to be

$$\boxed{\mathrm{i}u_t = [-\Delta + V(\mathbf{r})]u.} \qquad (2)$$

Imaginary numbers! It was a new departure for i to appear in one of the fundamental laws of physics. What is observed in the laboratory must of course be real, and here is the interpretation of the variable u: $u(\mathbf{r},t)$ is not observable, but the square of its absolute value, $|u(\mathbf{r},t)|^2$, is observable as the *probability density per unit volume* for the particle to appear at position $\mathbf{r}$ at time t. Thus at each time t, the integral of $|u|^2$ over all space must be equal to 1, and by integrating (2) by parts one can confirm that if this condition condition holds for $t = 0$, then it holds for $t > 0$.

Solutions to Schrödinger's equation are wavelike. For simplicity let us consider the 1D special case of (2) with $V(x) = V = \text{const}$,

$$\mathrm{i}u_t = -u_{xx} + Vu. \qquad (3)$$

For any *frequency* $\omega \in \mathbb{R}$, this equation admits the solution

$$u(x,t) = e^{i(kx-\omega t)} \qquad (4)$$

provided the *wave number* k is one of the two solutions of the *dispersion relation*

$$\omega = k^2 + V. \qquad (5)$$

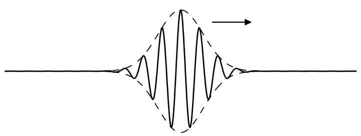

Fig. 1: 1D wave packet

For $\omega < V$, the two allowed values of k are imaginary and we have evanescent solutions that decrease exponentially as x increases or decreases. For $\omega > V$, they are real, and we have oscillatory wave solutions. A typical solution of this kind would be a *wave packet* formed by superposition of various Fourier modes (4) with central wave number k, phase velocity $c = \omega/k$ and group velocity $C = \mathrm{d}\omega/\mathrm{d}k$. In Fig. 1 the dashed line is $\pm|u(x)|$ and the solid line is $\mathrm{Re}\,u(x)$.

For particles of macroscopic mass, because $\hbar$ is so small, k and ω are normally huge and the wave packet behaves like a particle. For example, a tennis ball being served corresponds to a wave packet with wavelength on the order of 10^{-31} cm and frequency on the order of 10^{33} Hz.

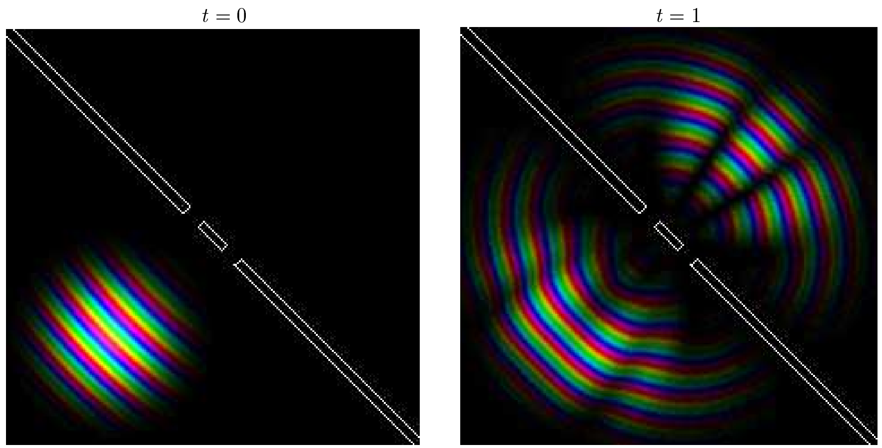

Fig. 2: 2D wave packet passing through a pair of slits

For microscopic particles, the wave nature of solutions to (2) becomes crucial. A famous example is the phenomenon of *quantum interference*. For example, Fig. 2 shows a wave packet in 2D propagating toward a barrier with two slits; the colors depict real and imaginary parts. This might be an electron emitted from a cathode ray tube. Mathematically, we have a potential in (2) with $V(\mathbf{r}) = 0$ in most of $\mathbb{R}^2$ but $V(\mathbf{r}) = \infty$ in the barrier regions. After impact, the wave packet has amplitude on both sides of the barrier. The particle has simultaneously passed through the slits and been reflected! Moreover, dark bands in the transmitted and reflected waves show regions where the portions of the wave passing through the slits have approximately canceled and the probability density is close to zero. These effects have no counterparts in classical mechanics.

Another effect explained by Schrödinger's equation is *tunneling*, which makes radioactive elements radioactive. This phenomenon depends on the evanescent portions of solutions to (2) or (3), which imply that inside a potential barrier of finite height, the wave function decays exponentially but is not zero. If the barrier has finite width, some amount of probability leaks through.

References

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