

Derivation Analytical Solution

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1 One-dimensional Schrödinger Equation

The one-dimensional Schrödinger equation for a free particle in natural units is

$$-\frac{1}{2}\partial_x^2\Psi(x,t) = i\partial_t\Psi(x,t). \quad (1)$$

Transforming into momentum-space yields the PDE

$$-\frac{1}{2}(ik)^2\tilde{\Psi}(k,t) = i\partial_t\tilde{\Psi}(k,t),$$

with solution

$$\tilde{\Psi}(k,t) = g(k) \exp\left(-i\frac{k^2t}{2}\right).$$

The spatial wavefunction $\Psi(x,t)$ that solves (1) can be recovered from its momentum-space representation via an inverse Fourier transform:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) \exp\left(i\left[kx - \frac{k^2t}{2}\right]\right) dk \quad (2)$$

From the above, the coefficient function $g(k)$ can be identified as the Fourier transform of the initial condition $\Psi(x,0)$ into momentum-space:

$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) \exp(-ikx) dx. \quad (3)$$

Thus, solving the PDE (1) for a given initial condition $\Psi(x,0)$ requires evaluating the two integrals (3) and (2).

Given the initial condition

$$\Psi(x,0) = \left(\frac{2a}{\pi}\right)^{1/4} \exp(-ax^2 + ik_0x) \quad (4)$$

the function $g(k)$ corresponding to this travelling Gaussian wavepacket is

$$\begin{aligned}
g(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[\left(\frac{2a}{\pi} \right)^{1/4} \exp(-ax^2 + ik_0x) \right] \exp(-ikx) dx \\
&= \left(\frac{a}{2\pi^3} \right)^{1/4} \int_{-\infty}^{\infty} \exp(-ax^2 - i[k - k_0]x) dx \\
&= \left(\frac{a}{2\pi^3} \right)^{1/4} \int_{-\infty}^{\infty} \exp \left(- \left[\left(\sqrt{a}x + \frac{i(k - k_0)}{2\sqrt{a}} \right)^2 + \frac{(k - k_0)^2}{4a} \right] \right) dx \\
&= \left(\frac{a}{2\pi^3} \right)^{1/4} \exp \left(- \frac{[k - k_0]^2}{4a} \right) \int_{-\infty}^{\infty} \exp \left(- \left[\left(\sqrt{a}x + \frac{i(k - k_0)}{2\sqrt{a}} \right)^2 \right] \right) dx
\end{aligned}$$

The substitution $y = \left(\sqrt{a}x + \frac{i(k - k_0)}{2\sqrt{a}} \right)$ yields

$$g(k) = \left(\frac{a}{2\pi^3} \right)^{1/4} \exp \left(- \frac{[k - k_0]^2}{4a} \right) \int_{-\infty}^{\infty} \frac{1}{\sqrt{a}} \exp(-y^2) dy.$$

Note that the standard Gaussian integral evaluates to

$$\int_{-\infty}^{\infty} \exp(-y^2) dy = \sqrt{\pi}$$

and hence we obtain

$$g(k) = \left(\frac{1}{2a\pi} \right)^{1/4} \exp \left(- \frac{[k - k_0]^2}{4a} \right). \quad (5)$$

Substituting this result into (2) yields

$$\begin{aligned}
\Psi(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{1}{2a\pi} \right)^{1/4} \exp \left(- \frac{[k - k_0]^2}{4a} + ikx - \frac{ik^2t}{2} \right) dk \\
&= \left(\frac{1}{8a\pi^3} \right)^{1/4} \int_{-\infty}^{\infty} \exp \left(-k^2 \left[\frac{1}{4a} + \frac{it}{2} \right] + k \left[\frac{k_0}{2a} + ix \right] - \frac{k_0^2}{4a} \right) dk
\end{aligned}$$

Defining appropriate parameters

$$\alpha = \left(\frac{1}{8a\pi^3} \right)^{1/4} \exp \left(- \frac{k_0^2}{4a} \right), \quad \beta^2 = \left[\frac{1}{4a} + \frac{it}{2} \right], \quad \gamma = \left[\frac{k_0}{2a} + ix \right]$$

the above can be re-written as

$$\begin{aligned}
\Psi(x, t) &= \alpha \int_{-\infty}^{\infty} \exp \left(-[\beta^2 k^2 - \gamma k] \right) dk \\
&= \alpha \int_{-\infty}^{\infty} \exp \left(- \left[\beta k - \frac{\gamma}{2\beta} \right]^2 + \frac{\gamma^2}{4\beta^2} \right) dk \\
&= \alpha \exp \left(\frac{\gamma^2}{4\beta^2} \right) \int_{-\infty}^{\infty} \exp \left(- \left[\beta k - \frac{\gamma}{2\beta} \right]^2 \right) dk
\end{aligned}$$

The substitution $K = \beta k + \frac{\gamma}{2\beta}$ yields

$$\Psi(x, t) = \frac{\alpha}{\beta} \exp\left(\frac{\gamma^2}{4\beta^2}\right) \int_{-\infty}^{\infty} e^{-K^2} dK = \sqrt{\pi} \frac{\alpha}{\beta} \exp\left(\frac{\gamma^2}{4\beta^2}\right).$$

Thus, the solution to (1) with initial condition (4) is

$$\begin{aligned} \Psi(x, t) &= \sqrt{\pi} \left(\frac{1}{8a\pi^3}\right)^{1/4} \exp\left(-\frac{k_0^2}{4a}\right) \left(\frac{1}{4a} + \frac{it}{2}\right)^{-1/2} \exp\left(\frac{1}{4} \frac{\left[\frac{k_0}{2a} + ix\right]^2}{\left[\frac{1}{4a} + \frac{it}{2}\right]}\right) \\ &= \left(\frac{1}{8a\pi}\right)^{1/4} \left(\frac{1}{4a} + \frac{it}{2}\right)^{-1/2} \exp\left(\frac{1}{4} \frac{\left[\frac{k_0}{2a} + ix\right]^2}{\left[\frac{1}{4a} + \frac{it}{2}\right]} - \frac{k_0^2}{4a}\right) \\ &= \frac{\left(\frac{2a}{\pi}\right)^{1/4}}{\sqrt{1+2ita}} \exp\left(\frac{-ax^2 + ixk_0 + \frac{k_0^2}{4a} - \frac{k_0^2}{4a} - \frac{itk_0^2}{2}}{\sqrt{1+2ita}}\right) \end{aligned}$$

Hence, the analytical solution is

$$\boxed{\Psi(x, t) = \frac{1}{\sqrt{1+2ita}} \left(\frac{2a}{\pi}\right)^{1/4} \exp\left(\frac{-ax^2 + i\left[xk_0 - \frac{1}{2}k_0^2t\right]}{\sqrt{1+2ita}}\right)}.$$

2 Two-dimensional Schrödinger Equation

The two-dimensional Schrödinger equation for a free particle in natural units is

$$-\frac{1}{2}(\partial_x^2 + \partial_y^2)\Psi(x, y, t) = i\partial_t\Psi(x, y, t). \quad (6)$$

Transforming into momentum-space yields the PDE

$$-\frac{1}{2}([ik_x]^2 + [ik_y]^2)\tilde{\Psi}(k_x, k_y, t) = i\partial_t\tilde{\Psi}(k_x, k_y, t),$$

with solution

$$\tilde{\Psi}(k_x, k_y, t) = g_x(k_x)g_y(k_y) \exp\left(-i\frac{t}{2}[k_x^2 + k_y^2]\right).$$

The spatial wavefunction $\Psi(x, y, t)$ that solves (6) can be recovered from its momentum-space representation via an inverse Fourier transform:

$$\Psi(x, y, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g_x(k_x)g_y(k_y) \exp\left(i\left[k_x x + k_y y - \frac{t}{2}(k_x^2 + k_y^2)\right]\right) dk_x dk_y \quad (7)$$

From the above, the product $g_x(k_x)g_y(k_y)$ can be identified as the Fourier transform of the initial condition $\Psi(x, y, 0)$ into momentum-space:

$$g_x(k_x)g_y(k_y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi(x, y, 0) \exp(-i[k_x x + k_y y]) dx dy. \quad (8)$$

Thus, solving the PDE (6) for a given initial condition $\Psi(x, 0)$ requires evaluating the two integrals (8) and (7).

Given the initial condition

$$\Psi(x, y, 0) = \left(\frac{2a}{\pi}\right)^{1/4} \left(\frac{2b}{\pi}\right)^{1/4} \exp(-ax^2 - by^2 + i[k_{x0}x + k_{y0}y]) \quad (9)$$

the product $g_x(k_x)g_y(k_y)$ corresponding to this travelling Gaussian wavepacket is

$$g_x(k_x)g_y(k_y) = \left(\frac{1}{2a\pi}\right)^{1/4} \left(\frac{1}{2b\pi}\right)^{1/4} \exp\left(-\frac{[k_x - k_{x0}]^2}{4a} - \frac{[k_y - k_{y0}]^2}{4b}\right), \quad (10)$$

where the integral (8) was evaluated using the same techniques as in the one-dimensional case.

Substituting the above into (7) and generalising the methods applied in one dimension, we find

$$\Psi(x, y, t) = \frac{1}{\sqrt{(1 + 2ita)(1 + 2itb)}} \left(\frac{4ab}{\pi^2}\right)^{1/4} \exp\left(\frac{-ax^2 - by^2 + i[k_{x0}x + k_{y0}y - \frac{t}{2}(k_{x0}^2 + k_{y0}^2)]}{\sqrt{(1 + 2ita)(1 + 2itb)}}\right).$$