This paper deals with the free particle in quantum mechanics. It follows Griffiths, 2.4.

Hope I can help you learning quantum mechanics.

The time-independent Schrödinger equation for the free particle without any potential $V(x)$:

$$-\frac{\hbar^2}{2m}\cdot\frac{d^2}{dx^2}\psi(x) = E\cdot\psi(x)$$

We rearrange:

$$\frac{d^2}{dx^2}\psi(x) = -\frac{2m}{\hbar^2}\cdot E\cdot\psi(x)$$

We use $k^2 \equiv \frac{2mE}{\hbar^2}$, $k = \pm\frac{\sqrt{2mE}}{\hbar}$

$$\frac{d^2}{dx^2}\psi(x) = -k^2\cdot\psi(x)$$

Note: k depends of the energy.

Note: The energy can be any positive value, $E \geq 0$.

General Solution:

$$\psi(x) = A\cdot e^{ikx}$$

Note: Together with $\psi(x) = A\cdot e^{ikx}$ also $\psi(x) = B\cdot e^{-ikx}$ fulfills the differential equation $\frac{d^2}{dx^2}\psi(x) = -k^2\cdot\psi(x)$.

Using that every linear combination of possible solutions is a solution again we concentrate on $\psi(x) = A\cdot e^{ikx}$ with $-\infty < k < \infty$ making things easier.

$\psi(x) = A\cdot e^{ikx}$ is the stationary solution.

We add (multiply) the standard time dependence:

$$e^{-i\cdot\frac{E}{\hbar}\cdot t}$$

We use $\frac{\hbar^2 k^2}{2m} \equiv E$:

$$e^{-i\cdot\frac{E}{\hbar}\cdot t} \rightarrow e^{-i\cdot\frac{\hbar k^2}{2m}\cdot t}$$

We have:

$$\psi_k(x,t) = A\cdot e^{ikx}\cdot e^{-i\cdot\frac{\hbar k^2}{2m}\cdot t} = A\cdot e^{i\left(kx-\frac{\hbar k^2}{2m}\cdot t\right)}$$

This is a particular solution for a specific “energy” k.

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The wavelength:

$$\lambda = \frac{2\cdot\pi}{|k|}$$

The momentum according to de Broglie:

$$p = \hbar\cdot k$$

The range over all k gives the general solution:

$$\psi(x,t) = A\int_{-\infty}^{\infty}\phi(k)\cdot e^{i\left(kx-\frac{\hbar k^2}{2m}\cdot t\right)}dk$$

Note: This is a wave packet.

From this wave packet we get $\psi(x,0)$:

$$\psi(x,0) = A\int_{-\infty}^{\infty}\phi(k)\cdot e^{ikx}dk$$

We have to calculate $\phi(k)$.

This is made by Fourier transformation (Plancherel's theorem):

$$F(k) = \int_{-\infty}^{\infty}f(x)\cdot e^{-ikx}dx \Leftrightarrow f(x) = \frac{1}{2\pi}\cdot\int_{-\infty}^{\infty}F(k)\cdot e^{ikx}dk$$

Note: This is a method often used by physicists and mathematicians transforming a problem into a space (where it is easier to solve) and then transform it back to the original space.

With this method we get:

$$\phi(k) = \int_{-\infty}^{\infty}\psi(x,0)\cdot e^{-ikx}dx$$

The complete wave function:

$$\psi(x,t) = \frac{1}{2\pi}\cdot A\cdot\int_{-\infty}^{\infty}\phi(k)\cdot e^{i\left(kx-\frac{\hbar k^2}{2m}\cdot t\right)}dk$$

This expression shows: We have given a spatial distribution $\psi(x,0)$. We transform this by help of the Fourier transform into the energy space. The energy space is needed to bring dynamics into life and to get the time dependent wave function $\psi(x,t)$.

Example 1

A free particle initially localized in the range $-a < x < a$ at time $t = 0$:

$$\psi(x,0) = \begin{cases} A & -a < x < a \\ 0 & else \end{cases}$$

Note: $A, a \in \mathbb{R}, A, a > 0$

Step 1, normalization:

$$1 = \int_{-\infty}^{\infty}\psi(x,0)\psi^*(x,0)dx =$$

$$\int_{-a}^{a}(A\cdot A)dx = A^2\int_{-a}^{a}dx = 2\cdot a\cdot A^2$$

We get:

$$A = \frac{1}{\sqrt{2a}}$$

Step 2, calculation of $\phi(k)$:

$$\phi(k) = \frac{1}{\sqrt{2a}} \int_{-a}^{a} e^{-ikx} dx =$$

$$\frac{1}{\sqrt{2a}} \left| \frac{e^{-ikx}}{-ik} \right|_{-a}^{a} =$$

$$\frac{1}{\sqrt{2a}} \left(\frac{e^{-ika} - e^{ika}}{-ik} \right) =$$

$$\frac{1}{\sqrt{2a}} \left(\frac{-2 \cdot Im\left(e^{ika}\right)}{-ik} \right) =$$

$$\frac{1}{\sqrt{2a}} \left(\frac{-2 \cdot i \cdot sin(ka)}{-ik} \right) =$$

$$\frac{2}{k\sqrt{2a}} sin(ka) =$$

$$\frac{1}{k} \cdot \sqrt{\frac{2}{a}} \cdot sin(ka)$$

Step 3, the general solution:

$$\psi(x,t) = \frac{1}{2\pi} \cdot \frac{1}{k} \cdot \sqrt{\frac{2}{a}} \cdot \int_{-\infty}^{\infty} sin(ka) \cdot e^{i\left(kx - \frac{\hbar k^2}{2m} \cdot t\right)} dk =$$

$$\frac{1}{\pi} \cdot \frac{1}{k} \cdot \sqrt{\frac{1}{2a}} \cdot \int_{-\infty}^{\infty} sin(ka) \cdot e^{i\left(kx - \frac{\hbar k^2}{2m} \cdot t\right)} dk$$

Unfortunately, this integral cannot be solved analytically but numerically.

Example 2

The gaussian wave packet. A free particle has the initial wave function at time $t = 0$:

$$\psi(x,0) = A \cdot e^{-ax^2}$$

Note: $A, a \in \mathbb{R}, A, a > 0$

Step 1, normalization:

$$1 = \int_{-\infty}^{\infty} \psi(x,0)\psi^*(x,0)dx == A^2 \int_{-\infty}^{\infty} e^{-2ax^2} dx = A^2 \sqrt{\frac{\pi}{2a}}$$

$$A^2 = \left(\frac{2a}{\pi}\right)^{\frac{1}{2}} \rightarrow A = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}}$$

We get $\psi(x,0)$:

$$\psi(x,0) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \cdot e^{-ax^2}$$

Step 2, calculation of $\phi(k)$ according to Griffith, completing the square.

$$A^2 + 2AB + B^2 = (A+B)^2 \rightarrow$$

$$A^2 + 2AB = (A+B)^2 - B^2$$

We have the integral from the left, dealing with the exponent only:

$$\phi(k) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \int_{-\infty}^{\infty} e^{-(ax^2+ikx)} \cdot dx \rightarrow ax^2 + ikx$$

We set:

$$A^2 = ax^2 \rightarrow A = \sqrt{a}x$$

$$2AB = ikx$$

$$B^2 = ?$$

We calculate:

$$2AB = ikx = 2\sqrt{a}xB \rightarrow B = \frac{ikx}{2\sqrt{a}x} = \frac{ik}{2\sqrt{a}}$$

$$B^2 = \frac{k^2}{4a}$$

We get:

$$ax^2 + ikx = \left(\sqrt{a}x + \frac{ik}{2\sqrt{a}}\right)^2 - \frac{k^2}{4a}$$

We use:

$$y = \sqrt{a}x + \frac{ik}{2\sqrt{a}}$$

We need dx:

$$\frac{dy}{dx} = \sqrt{a} \rightarrow dx = \frac{dy}{\sqrt{a}}$$

We rewrite the integral:

$$\int_{-\infty}^{\infty} e^{-(ax^2+ikx)} \cdot dx = \int_{-\infty}^{\infty} e^{-y^2+\frac{k^2}{4a}} \cdot \frac{dy}{\sqrt{a}} =$$

$$\frac{1}{\sqrt{a}} \int_{-\infty}^{\infty} e^{-y^2+\frac{k^2}{4a}} \cdot dy = \frac{1}{\sqrt{a}} e^{\frac{k^2}{4a}} \cdot \sqrt{\pi} =$$

$$\sqrt{\frac{\pi}{a}} e^{\frac{k^2}{4a}}$$

Note: This is the result when you look at Wikipedia.

We get $\phi(k)$:

$$\phi(k) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \int_{-\infty}^{\infty} e^{-ax^2} \cdot e^{-ikx} dx =$$

$$\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\frac{\sqrt{\pi}}{\sqrt{a}}e^{-\frac{k^2}{4a}} = \left(\frac{2a\pi^2}{\pi a^2}\right)^{\frac{1}{4}}e^{-\frac{k^2}{4a}} =$$

$$\left(\frac{2\pi}{a}\right)^{\frac{1}{4}}e^{-\frac{k^2}{4a}}$$

Note: $\phi(k)$ is real function.

Step 3, the general solution.

We remember:

$$\psi(x,t) = \frac{1}{2\pi}\cdot A\cdot\int_{-\infty}^{\infty}\phi(k)\cdot e^{i\left(kx-\frac{\hbar k^2}{2m}\cdot t\right)}dk$$

We calculate:

$$\psi(x,t) = \frac{1}{2\pi}\cdot\left(\frac{2\pi}{a}\right)^{\frac{1}{4}}\cdot\int_{-\infty}^{\infty}e^{-\frac{k^2}{4a}}\cdot e^{i\left(kx-\frac{\hbar k^2}{2m}\cdot t\right)}dk =$$

$$\left(\frac{1}{2^3\pi^3 a}\right)^{\frac{1}{4}}\cdot\int_{-\infty}^{\infty}e^{-\frac{k^2}{4a}}\cdot e^{i\left(kx-\frac{\hbar k^2}{2m}\cdot t\right)}dk =;$$

We calculate the exponent:

$$e^{-\frac{k^2}{4a}}\cdot e^{i\left(kx-\frac{\hbar k^2}{2m}\cdot t\right)} =$$

$$\exp\left(-\frac{k^2}{4a}+ikx-i\frac{\hbar k^2}{2m}\cdot t\right) =$$

$$exp-\left(k^2\left(\frac{1}{4a}+\frac{i\hbar}{2m}\cdot t\right)-ikx\right)$$

We proceed:

$$\left(\frac{1}{2^3\pi^3 a}\right)^{\frac{1}{4}}\cdot\int_{-\infty}^{\infty}e^{-\left(k^2\left(\frac{1}{4a}+\frac{i\hbar}{2m}\cdot t\right)-ikx\right)}dk =;$$

We have the coefficient with k^2:

$$\left(\frac{1}{4a}+\frac{i\hbar}{2m}\cdot t\right)$$

We have the coefficient with k:

$$-ix$$

We get the value of the integral (Wikipedia):

$$\sqrt{\frac{\pi}{\frac{1}{4a}+\frac{i\hbar}{2m}\cdot t}}\cdot e^{\left(-\frac{x^2}{\frac{1}{a}+\frac{2i\hbar}{m}\cdot t}\right)}$$

We calculate $\psi(x,t)$:

$$\left(\frac{1}{2^3\pi^3 a}\right)^{\frac{1}{4}}\cdot\sqrt{\frac{\pi}{\frac{1}{4a}+\frac{i\hbar}{2m}\cdot t}}\cdot e^{\left(-\frac{x^2}{\frac{1}{a}+\frac{2i\hbar}{m}\cdot t}\right)}=$$

$$\left(\frac{1}{2^3\pi^3 a}\right)^{\frac{1}{4}}\cdot\sqrt{\frac{\pi}{\frac{m+2ai\hbar t}{4am}}}\cdot e^{\left(-\frac{x^2}{\frac{1}{a}+\frac{2i\hbar}{m}\cdot t}\right)}=$$

$$\left(\frac{1}{2^3\pi^3 a}\right)^{\frac{1}{4}}\cdot\sqrt{\frac{4am\pi}{m+2ai\hbar t}}\cdot e^{\left(-\frac{x^2}{\frac{1}{a}+\frac{2i\hbar}{m}\cdot t}\right)}=$$

$$\left(\frac{2^4a^2\pi^2}{2^3\pi^3 a}\right)^{\frac{1}{4}}\cdot\sqrt{\frac{m}{m+2ai\hbar t}}\cdot e^{\left(-\frac{x^2}{\frac{1}{a}+\frac{2i\hbar}{m}\cdot t}\right)}=$$

$$\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\cdot\frac{e^{\left(-\frac{x^2}{\frac{1}{a}+\frac{2i\hbar}{m}\cdot t}\right)}}{\sqrt{1+\frac{2ai\hbar t}{m}}}$$

Result:

$$\psi(x,t)=\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\cdot\frac{e^{\left(-\frac{ax^2}{1+\frac{2ai\hbar t}{m}}\right)}}{\sqrt{1+\frac{2ai\hbar t}{m}}}$$

We calculate $|\psi(x,t)|^2=\psi(x,t)\psi^*(x,t)$:

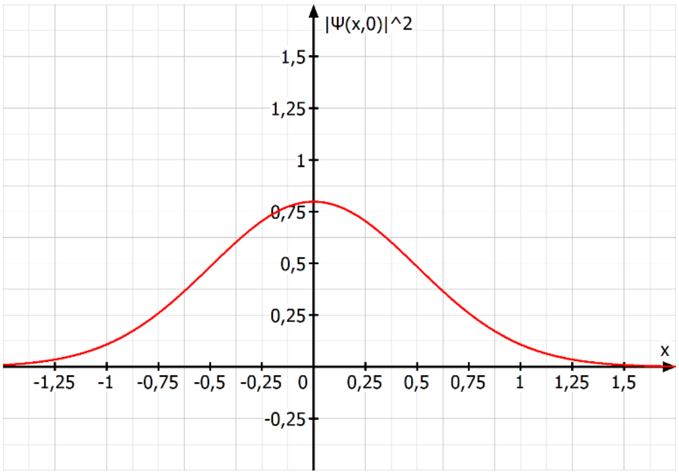
$$\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\cdot\frac{e^{\left(-\frac{ax^2}{1+\frac{2ai\hbar t}{m}}\right)}}{\sqrt{1+\frac{2ai\hbar t}{m}}}\cdot\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\cdot\frac{e^{\left(-\frac{ax^2}{1-\frac{2ai\hbar t}{m}}\right)}}{\sqrt{1-\frac{2ai\hbar t}{m}}}=$$

$$\left(\frac{2a}{\pi}\right)^{\frac{1}{2}}\cdot\frac{e^{-ax^2\left(\frac{1}{1+\frac{2ai\hbar t}{m}}+\frac{1}{1-\frac{2ai\hbar t}{m}}\right)}}{\sqrt{1+\left(\frac{2a\hbar t}{m}\right)^2}}=$$

$$\left(\frac{2a}{\pi}\right)^{\frac{1}{2}}\cdot\frac{e^{-2ax^2\left(\frac{1}{1+\left(\frac{2a\hbar t}{m}\right)^2}\right)}}{\sqrt{1+\left(\frac{2a\hbar t}{m}\right)^2}}$$

We plot $|\psi(x,t)|^2$ for $t = 0$ and $a = 1$:

$$|\psi(x,t)|^2{}_{t=0} = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \cdot e^{-2x^2}$$



Note: For $t = 0$ $\hbar, m$ vanish with the exception $m \neq 0$.

We plot $|\psi(x,t)|^2$ for $t = 10$ and $a, \hbar, m = 1$:

$$|\psi(x,t)|^2{}_{t=10} = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \cdot \frac{e^{-2x^2\left(\frac{1}{1+(20)^2}\right)}}{\sqrt{1+(20)^2}}$$