Lösung der Schrödinger- Gleichung für ein freies Teilchen.

Gegeben ist die Schrödinger Gleichung in stationärer Form:

$$-\frac{\hbar^2}{2m}\phi'' + E_{pot}\phi = E\phi$$

Es soll ein freies Teilchen vorliegen:

$$E_{pot} = 0$$

$\Rightarrow$

$$\frac{\hbar^2}{2m}\phi'' + E\phi = 0$$

$\Rightarrow$

$$\phi'' + \frac{2m}{\hbar^2}E\phi = 0$$

Lösung durch den Ansatz nach „Allgemeine, homogene, lineare Differentialgleichung 2. Ordnung“. Die Charakteristische Gleichung:

$$\lambda^2 + \frac{2m}{\hbar^2}E = 0$$

$\Rightarrow$

$$\lambda_{1;2} = \pm\sqrt{-\frac{2m}{\hbar^2}E}$$

$\Rightarrow$

$$a \pm ib = 0 \pm i\sqrt{\frac{2m}{\hbar^2}E}$$

Schwingungsfähig dann, wenn gilt:

$$\frac{2m}{\hbar^2}E > 0$$

Ist immer erfüllt. Die Lösung lautet daher:

$$\phi = \sin(bx)$$

$\Rightarrow$

$$\phi = \sin\left(\frac{x}{\hbar}\sqrt{2mE}\right)$$

mit:

$$b=\omega_x=\sqrt{\frac{2m}{\bar{h}^2}E}\left[\sqrt{\frac{kg}{J^2s^2}J}=\sqrt{\frac{kg}{Nms^2}}=\sqrt{\frac{kgs^2}{kgm^2s^2}}=\sqrt{\frac{1}{m^2}}=\frac{1}{m}\right]$$

$\Rightarrow$

$$\omega_x=\frac{\sqrt{2mE}}{\bar{h}}$$

$\Rightarrow$

$$f_x=\frac{1}{h}\sqrt{2mE}\left[\frac{1}{Js}\sqrt{kgJ}=\frac{1}{Nms}\sqrt{kgNm}=\frac{s^2}{kgm^2s}\sqrt{kg\frac{kgm}{s^2}m}=\frac{skgm}{kgm^2s}=\frac{1}{m}\right]$$

Kontrolle der Lösung:

$$\phi=\sin\left(\frac{x}{\bar{h}}\sqrt{2mE}\right)$$
$$\phi'=\frac{\sqrt{2mE}}{\bar{h}}\cos\left(\frac{x}{\bar{h}}\sqrt{2mE}\right)$$
$$\phi''=-\frac{2mE}{\bar{h}^2}\sin\left(\frac{x}{\bar{h}}\sqrt{2mE}\right)$$

$\Rightarrow$

$$\phi''+\frac{2m}{\bar{h}^2}E\phi=0$$

$\Rightarrow$

$$-\frac{2m}{\bar{h}^2}E\sin\left(\frac{x}{\bar{h}}\sqrt{2mE}\right)+\frac{2m}{\bar{h}^2}E\sin\left(\frac{x}{\bar{h}}\sqrt{2mE}\right)=0$$

$\Rightarrow$

$$0=0$$

Die Lösung ist exakt, jedoch muss gelten:

$$C\int_{-\infty}^{+\infty}\phi\bar{\phi}dx=1$$

$\Rightarrow$

$$\phi=\sin\left(\frac{x}{\bar{h}}\sqrt{2mE}\right)=\sin kx$$

In Komplexschreibweise:

$$\phi=\sin kx=\cos kx+i\sin kx$$

$\Rightarrow$

$$\phi=\cos kx+i\sin kx=e^{ikx}$$

$\Rightarrow$

$$\overline{\phi} = e^{-ikx}$$

$\Rightarrow$

$$\phi\overline{\phi} = e^{ikx}e^{-ikx} = e^{0} = 1$$

$\Rightarrow$

$$C\int_{0}^{L} dx = 1$$

$\Rightarrow$

$$C = \frac{1}{L} \rightarrow \lim_{L\rightarrow\pm\infty} = 0$$

Wobei „L“ die betrachtete Weglänge darstellt. Das Teilchen hält sich unabhängig von seiner Geschwindigkeit überall und ständig mit gleicher Wahrscheinlichkeit auf. Der Ort ist völlig unbestimmt.

Daher gilt endgültig:

$$\phi = \sin\left(\frac{x}{\overline{h}}\sqrt{2mE}\right)\left[\frac{m}{Js}\sqrt{kgJ} = \frac{m}{Nms}\sqrt{kgNm} = \frac{s}{kgm}\sqrt{\frac{kg^{2}m^{2}}{s^{2}}} = 1\right]$$

Wobei die Energie der freien Welle die kinetische Energie ist:

$$E = \frac{p^{2}}{2m}$$

$\Rightarrow$

$$\phi = \sin\left(x\sqrt{\frac{2m}{\overline{h}^{2}}\frac{p^{2}}{2m}}\right)$$

$\Rightarrow$

$$\boxed{\phi(x) = \sin\left(\frac{p}{\overline{h}}x\right)\left[\frac{Ns}{Js}m = \frac{N}{Nm}m = 1\right]}$$

Wobei „p“ den Impuls des Teilchens darstellt.

$$\boxed{\omega(x) = \frac{p}{\overline{h}}\left[\frac{Ns}{Js} = \frac{N}{Nm} = \frac{1}{m}\right]}$$

$\Rightarrow$

$$f_{x} = \frac{p}{h}\left[\frac{Ns}{Js} = \frac{N}{Nm} = \frac{1}{m}\right]$$

Die de- Broglie- Relation:

$$p = \frac{h}{\lambda} = k\bar{h}$$

$\Rightarrow$

$$\phi = \sin\frac{p}{\bar{h}}x = \sin\frac{2\pi}{\lambda}x$$

Die Wellenlänge- Frequenz- Relation:

$$\lambda = \frac{c}{f_t}$$

$\Rightarrow$

$$\phi = \sin\frac{2\pi}{c}f_t x$$

Die Definition der Kreisfrequenz:

$$\omega = \omega_t = 2\pi f_t = 2\pi\frac{c}{\lambda} = \frac{cp}{\bar{h}}$$

$\Rightarrow$

$$\phi = \sin\frac{\omega}{c}x$$

Die Definition der nichtrelativistischen Geschwindigkeit:

$$c = \frac{x}{t}$$

$\Rightarrow$

$$\boxed{\phi(t) = \sin\omega t\left[\frac{1}{s}s = 1\right]}$$

Die Energie für eine Welle:

$$\boxed{E = \bar{h}\,\omega\left[J\frac{s}{s} = J\right]}$$

Mit:

$$\boxed{\omega(t) = \frac{p}{\bar{h}}c\left[\frac{mNs}{sJs} = \frac{mN}{sNm} = \frac{1}{s}\right]}$$

Der Übergang zur zeitabhängigen Schrödinger- Gleichung erfolgt durch:

$$\psi(x;t) = \phi(x) e^{-\frac{i}{\hbar}Et}$$

$\Rightarrow$

$$\psi(x;t) = \phi(x) e^{-i\omega_t t}$$

$\Rightarrow$

$$\psi(x;t) = \sin(\omega_x x) e^{-i\omega_t t}$$

$\Rightarrow$

$$\psi(x;t) = \sin(\omega_x x)[\cos(\omega_t t) - i\sin(\omega_t t)]$$

$\Rightarrow$

$$\psi(x;t) = \sin(\omega_x x)\cos(\omega_t t) - i\sin(\omega_x x)\sin(\omega_t t)$$

Es erfolgt eine Zerlegung in Real- und Imaginäranteil:

$$\Re\psi = \sin(\omega_x x)\cos(\omega_t t)$$
$$\Im\psi = -\sin(\omega_x x)\sin(\omega_t t)$$

Die Ergebnisse werden den Achsen eines kartesischen Koordinaten-systems zugeordnet und in polare umgewandelt:

$$x(\psi) = \Re\psi$$
$$y(\psi) = \Im\psi$$

$\Rightarrow$

$$x(\psi) = \sin(\omega_x x)\cos(\omega_t t)$$
$$y(\psi) = -\sin(\omega_x x)\sin(\omega_t t)$$

$\Rightarrow$

$$x(\psi)^2 + y(\psi)^2 = \sin^2(\omega_x x)\left(\cos^2(\omega_t t) + \sin^2(\omega_t t)\right)$$
$$\frac{y}{x}(\psi) = -\frac{\sin(\omega_t t)}{\cos(\omega_t t)}$$

$\Rightarrow$

$$r = \sqrt{x(\psi)^2 + y(\psi)^2} = \sin(\omega_x x)$$
$$\tan\varphi = \frac{y}{x}(\psi) = -\tan(\omega_t t)$$

$\Rightarrow$

$$r = \sin(\omega_x x)$$
$$\varphi = -\omega_t t$$

Es wurde berechnet:

$$\omega(x) = \frac{p}{\hbar}$$

$$\omega(t) = \frac{p}{\hbar} c$$

$\Rightarrow$

$$\omega(t) = c\,\omega(x)$$

$\Rightarrow$

$$r = \sin(\omega_x x)$$
$$\varphi = -c\,\omega_x t$$

Sowie:

$$ct = x$$

$\Rightarrow$

$$r(x) = \sin(\omega_x x)$$
$$\varphi(x) = -\omega_x x$$

$\Rightarrow$

$$r(\varphi) = -\sin\varphi$$

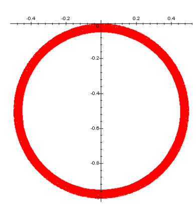
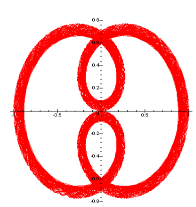
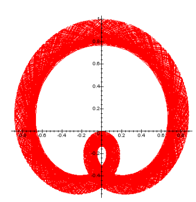
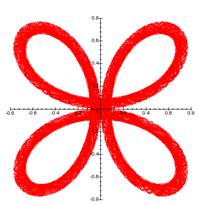
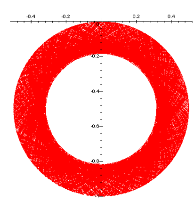
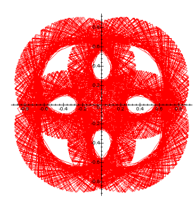
Oder man wählt folgende Umformung zwecks graphischer Veranschaulichung:

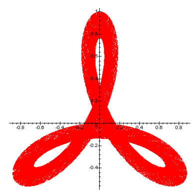
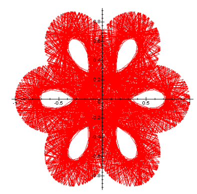
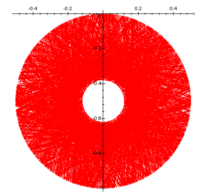
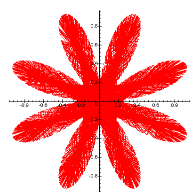
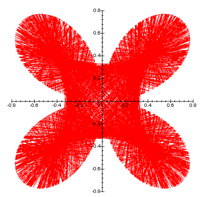
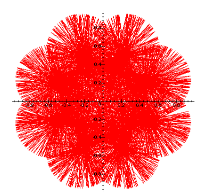
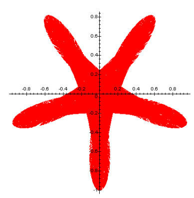
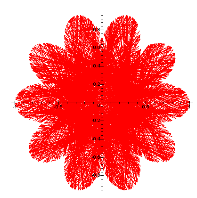
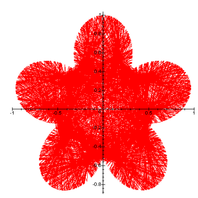
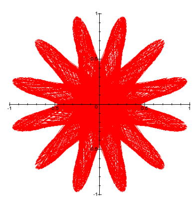
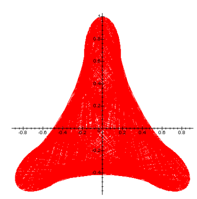
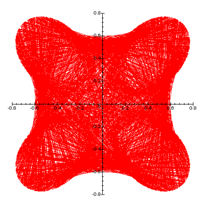
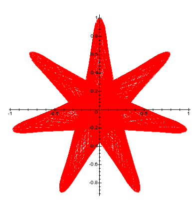
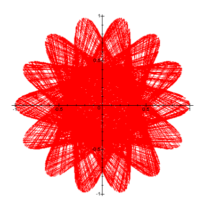
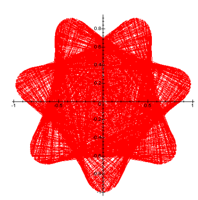
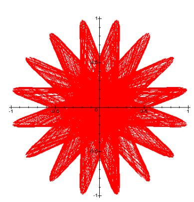
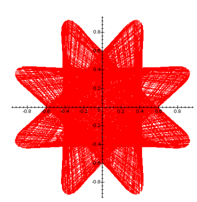
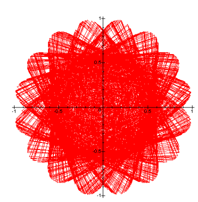
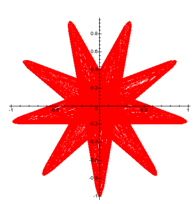
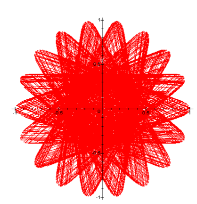
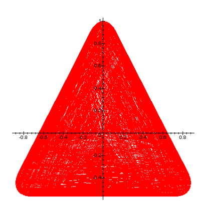
$$ct = x$$

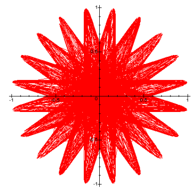
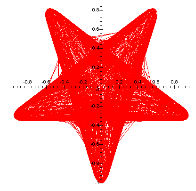
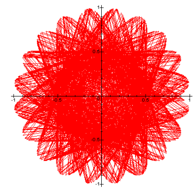
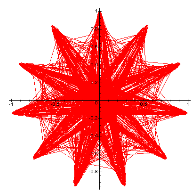
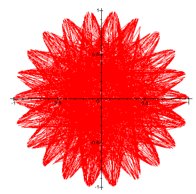
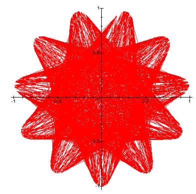
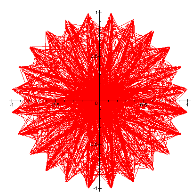
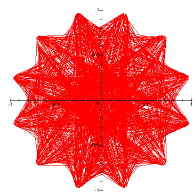
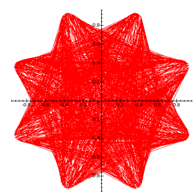
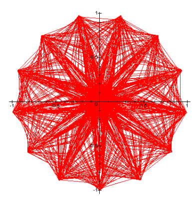
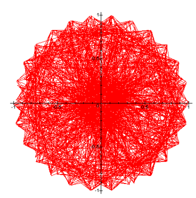
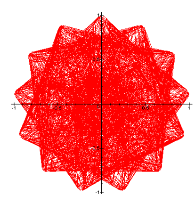
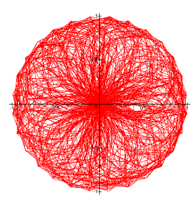
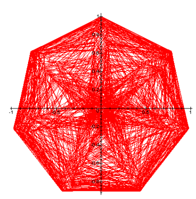
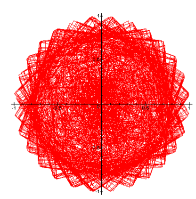
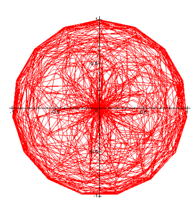
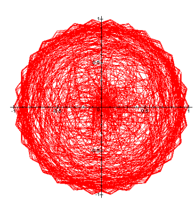
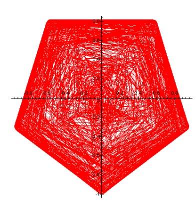
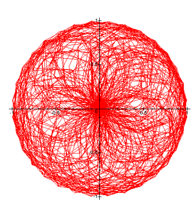
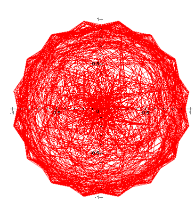
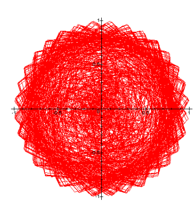
$\Rightarrow$

$$r(t) = \sin(\omega_x ct)$$
$$\varphi(t) = -\omega_t t$$

In Polarkoordinatendarstellung ergeben sich folgende Schaubilder:

t = 0..1	$\omega_t = 200\pi$	$\omega_t = 400\pi$	$\omega_t = 800\pi$
$\omega_x c = 200\pi$			
$\omega_x c = 400\pi$			

$\omega_x c = 600\pi$			
$\omega_x c = 800\pi$			
$\omega_x c = 1000\pi$			
$\omega_x c = 1200\pi$			
$\omega_x c = 1400\pi$			
$\omega_x c = 1600\pi$			
$\omega_x c = 1800\pi$			

$\omega_x c = 2000\pi$			
$\omega_x c = 2200\pi$			
$\omega_x c = 2400\pi$			
$\omega_x c = 2600\pi$			
$\omega_x c = 2800\pi$			
$\omega_x c = 3000\pi$			
$\omega_x c = 3200\pi$			

Wobei nun der Bereich des physikalischen Begriffs der Einteilchen-Wellenfunktionen - Orbitale beginnt.