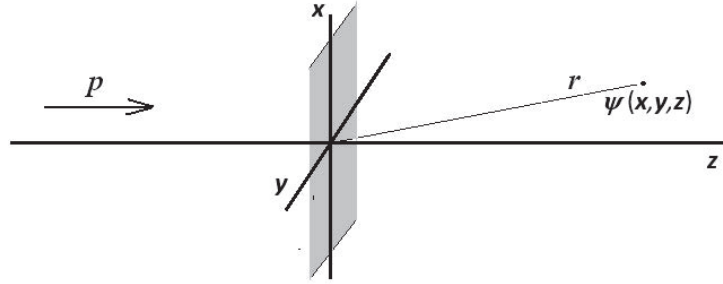


Derivation of Huygen's principle from the time-independent Schrodinger equation

Here we discuss a non-normalizable energy eigenstate solving the time-independent Schrodinger equation that describes a particle with momentum $\vec{p} = p\hat{z}$ incident from the left on a translucent screen and show how the resulting wave function on the right of the screen can be obtain using Huygen's principle.



Assume that the translucent screen is placed in the plane described by the coordinates $(x, y, z = 0)$ and that that for $z < 0$ the energy eigenstate contains the plane wave $\exp\{ip\hat{z}/\hbar\}$ which describes a particle moving in the $+\hat{z}$ direction where $\hat{z}$ is a unit vector pointing in the positive z direction. For $z < 0$ the solution should be a combination of this incoming plane wave and a scattered wave which is not the objective of this discussion. We will assume that immediately on the positive z side of the translucent screen the wave function has the form:

$$\psi(x, y, z) = \phi(x, y)e^{ipz/\hbar} \quad \text{for } z \approx 0. \quad (1)$$

Here the x and y dependence introduced by the factor $\phi(x, y)$ is intended to be the effect of the screen which transmits the quantum wave in a fashion that depends on x and y .

We assume that the only non-zero potential which affects our particle is localized at the $z = 0$ position of the screen, for $z \neq 0$ we should require that $\psi(x, y, z)$ obey the time-independent Schrodinger equation for a particle of energy E :

$$\frac{(-i\hbar\vec{\nabla})^2}{2m}\psi(x, y, z) = E\psi(x, y, z) \quad \text{for } z \neq 0. \quad (2)$$

This equation is obeyed by the incoming plane wave given by $\exp\{ip\hat{z}/\hbar\}$ which is assumed to be one of the terms contributing to the wave function $\psi(x, y, z)$ on the left hand side of the screen. This implies that $E = \vec{p}^2/2m$. The effects of the translucent screen are described by the wavefunction immediately to the right-hand side of the barrier and act as a boundary condition that must be obeyed by the solution $\psi(x, y, z)$ for $z > 0$ in which we are interested. Thus, the problem is to determine $\psi(x, y, z)$ for $z > 0$ in terms of functions $\psi(x, y, 0)$ and $(\partial\psi(x, y, z)/\partial z)_{z=0}$ – a natural application for Green's functions methods.

Recall that a Green's functions that are used to solve the time-independent Schrodinger equation is

$$G(\vec{r}) = \frac{1}{4\pi} \frac{e^{ipr/\hbar}}{r} \quad (3)$$

which obeys the equation:

$$\left\{ \nabla^2 + \frac{2m}{\hbar^2} E \right\} G(\vec{r}) = -\delta^3(\vec{r}) \quad (4)$$

where

$$\vec{\nabla}^2 = \sum_{i=1}^3 \frac{\partial^2}{\partial r_i^2}. \quad (5)$$

[You should be able to derive Eq. (4) from the more familiar equation that underlies the Poisson's equation obeyed by the electrostatic potential created by a point charge: $\vec{\nabla}^2(1/r) = -4\pi\delta^3(\vec{r})$.] The following application of Gauss' theorem uses $G(\vec{r})$ to determine $\psi(\vec{r})$ in a 3-dimensional volume V in terms of its values on the boundary, ∂V , of the volume V in the case that $\psi(\vec{r})$ obeys the Schrodinger equation with no potential term inside the volume V .

We begin with the equation:

$$\psi(\vec{r}) = \int_V d^3r' \vec{\nabla}_{r'} \cdot \left\{ \left[\vec{\nabla}_{r'} \psi(\vec{r}') \right] G(\vec{r} - \vec{r}') - \left[\vec{\nabla}_{r'} G(\vec{r} - \vec{r}') \right] \psi(\vec{r}') \right\}. \quad (6)$$

where the gradient produces four terms when it acts on the two products that are subtracted inside the curly brackets. Two of those term are identical and cancel. The other two terms where $\vec{\nabla}^2$ acts on one of the two functions would also be the same and cancel if $\psi(\vec{r}')$ and $G(\vec{r}' - \vec{r})$ both obeyed the time-independent Schrodinger equation with energy E . This is true, except for the δ function in Eq. (??) and it is this term that provides the left-hand side of Eq. (6).

In the next step we apply Gauss' theorem to Eq. (6) writing the volume integral of the divergence as equal to the surface integral of the normal component of the vector whose divergence is being taken:

$$\psi(\vec{r}) = \int_{\partial V} dS' \hat{n} \cdot \left\{ \left[\vec{\nabla}_{r'} \psi(\vec{r}') \right] G(\vec{r} - \vec{r}') - \left[\vec{\nabla}_{r'} G(\vec{r} - \vec{r}') \right] \psi(\vec{r}') \right\}. \quad (7)$$

Since in our application the volume V is the entire $z > 0$ region we can neglect the surface at $z \rightarrow \infty$ and keep only the $z = 0$ surface where we obtain the relation we need:

$$\begin{aligned} \psi(\vec{r}) = \iint dx' dy' \left\{ \left[\frac{\partial}{\partial z'} \psi(x', y', z') \right]_{z'=0} G(x - x', y - y', -z) \right. \\ \left. - \left[\frac{\partial}{\partial z'} G(\vec{r} - \vec{r}') \right]_{z'=0} \psi(x', y', 0) \right\}. \end{aligned} \quad (8)$$

This very general equation can be put into a simpler form if we assume that our translucent screen becomes opaque for $\sqrt{(x')^2 + (y')^2} > R$ for some large, fixed radius R and then examine the right-hand side, $\psi(\vec{r})$ for $r \gg R$.

With this approximation we can examine $G(\vec{r} - \vec{r}')$ in Eq. (3):

$$\frac{1}{4\pi} \frac{e^{ip|\vec{r}-\vec{r}'|/\hbar}}{|\vec{r}-\vec{r}'|} \approx \frac{1}{4\pi r} e^{ipr\sqrt{1-2\hat{r}\cdot\vec{r}'}/\hbar} \quad (9)$$

$$\approx \frac{e^{ipr/\hbar}}{4\pi r} e^{-i\vec{p}\cdot\vec{r}'/\hbar} \quad (10)$$

where the vector $\vec{p}$ is in the direction of the vector $\vec{r}$ but with the magnitude p :

$$\vec{p} = p\hat{r}. \quad (11)$$

If Equation (10) is substituted into Eq. (8), we recognize that we are performing a two-dimensional Fourier transform of $\psi(x', y', 0)$ with respect to the two-dimensional momentum $\vec{p}_\perp = p[(\hat{r})_x + (\hat{r})_y]$. We must now determine both of the two terms in Eq. (8). The right-most term on the right hand side of Eq. (8) is easy to evaluate, since:

$$\left[\frac{\partial}{\partial z'} G(\vec{r} - \vec{r}') \right]_{z'=0} = -ip_z/\hbar = -ip\hat{r}_z\hbar \approx -ip/\hbar \quad (12)$$

if we assume that we are evaluating $\psi(\vec{r})$ where $\vec{r}$ makes a small angle with the z axis. Note this “small angle” approximation is a second approximation, in addition to our long-distance assumption $r \gg R$ introduced on the previous page.

The other term on the right-hand side of Eq. (8) is not more difficult to determine if we continue with this small angle approximation. We need to determine

$$\frac{\partial}{\partial z'} \left\{ \iint dx' dy' \psi(x', y', z') \exp^{-i(\vec{p}_\perp \cdot \vec{r}')/\hbar} \right\}_{z'=0} \quad (13)$$

We can use the free Schrodinger equation to evaluate the related quantity:

$$\frac{\partial^2}{\partial (z')^2} \left\{ \iint dx' dy' \psi(x', y', z') \exp^{-i(\vec{p}_\perp \cdot \vec{r}')/\hbar} \right\}_{z'=0} \quad (14)$$

$$\begin{aligned} &= \iint dx' dy' \exp^{-i(\vec{p}_\perp \cdot \vec{r}')/\hbar} \left[-\left(\frac{p}{\hbar}\right)^2 - \frac{\partial^2}{\partial (x')^2} - \frac{\partial^2}{\partial (y')^2} \right] \psi(x', y', z') \\ &= \left(\frac{-p^2 + \vec{p}_\perp^2}{\hbar^2} \right) \iint dx' dy' \exp^{-i(\vec{p}_\perp \cdot \vec{r}')/\hbar} \psi(x', y', z'=0) \end{aligned} \quad (15)$$

for $z' > 0$ and close to 0. Since our small-angle approximation guarantees that $|\vec{p}_\perp| \ll p$, we can neglect $\vec{p}_\perp^2$ when subtracted from p^2 and derive the differential equation:

$$\frac{\partial^2}{\partial (z')^2} \left\{ \iint dx' dy' \psi(x', y', z') \exp^{-i(\vec{p}_\perp \cdot \vec{r}')/\hbar} \right\} \quad (16)$$

$$= -\frac{p^2}{\hbar^2} \left\{ \iint dx' dy' \exp^{-i(\vec{p}_\perp \cdot \vec{r}')/\hbar} \psi(x', y', z') \right\} \quad (17)$$

with the solutions

$$\iint dx' dy' \psi(x', y', z') \exp^{-i(\vec{p}_\perp \cdot \vec{r}')/\hbar} \quad (18)$$

$$= e^{\pm ipz/\hbar} \iint dx' dy' \exp^{-i(\vec{p}_\perp \cdot \vec{r}')/\hbar} \psi(x', y', 0) \quad (19)$$

Since there is no left-moving wave on the right-hand side of the screen we can discard the $\exp -ipz/\hbar$ solution in Eq. (19) and can now evaluate the left-most term on the right-hand side of Eq. (8), find the same result as we found for the right hand term, simply doubling the result. Thus, Eq. (8) becomes

$$\psi(\vec{r}) = \frac{ipe^{ipr}}{2\pi r\hbar} \left\{ \iint dx' dy' \exp^{-i(\vec{p}_\perp \cdot \vec{r}')/\hbar} \psi(x', y', z') \right\}. \quad (20)$$

This is the result we obtained from our Huygen's principle approach but now with a known proportionality constant. This is known as the Rayleigh-Sommerfeld formula.

Acknowledgement

ChatGPT suggested using Eq. (7) but was unable to appropriately approximate its right-hand side.