Wave velocity and group velocity

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1 General wave packets

Suppose we have a wave packet centered smoothly around some large value of k, say k_0 given by a superposition of plane waves

$$e^{i(kx-\omega t)}$$

A peak of the real part of the wave corresponds to $kx - \omega t = 2n\pi$ and will appear to move with velocity

$$\begin{aligned} v_{phase} &= \frac{dx}{dt} \\ &= \frac{1}{k}\frac{d\left(2\pi n + \omega t\right)}{dt} \\ &= \frac{\omega}{k} \\ &= \frac{2\pi f}{2\pi/\lambda} \\ &= \lambda f \end{aligned}$$

This is called the *phase velocity* of the wave; it is the speed of a point of fixed phase. This is not the speed at which the wave packet formed by a superposition travels.

Let the packet be described by a smooth distribution $A(k)$ (for example, a Gaussian),

$$\begin{aligned} \Psi(x,t) &= \int dk A(k)\, e^{\frac{i}{\hbar}(px-Et)} \\ &= \int dk A(k) \exp i\left(kx - \omega(k)\, t\right) \end{aligned}$$

and expand $\omega(k)$ in a Taylor series about k_0,

$$\omega(k) = \omega_0 + \left.\frac{d\omega}{dk}\right|_{k_0}(k-k_0) + \ldots$$

Substituting into the exponential,

$$\begin{aligned} \exp i\left(kx - \omega(k)\, t\right) &\approx \exp i\left(kx - \omega_0 t - \left.\frac{d\omega}{dk}\right|_{k_0} kt + \frac{d\omega}{dk}_{k_0} k_0 t\right) \\ &= \exp ik\left(x - \left.\frac{d\omega}{dk}\right|_{k_0} t\right)\exp -i\left(\omega_0 - \frac{d\omega}{dk}_{k_0} k_0\right)t \end{aligned}$$

where we separate out any terms that are independent of k. Then the integral becomes

$$\Psi(x,t) = \int dk A(k) \exp i\left(kx - \omega(k)\, t\right)$$

$$\approx \quad e^{-i\left(\omega_0-\frac{d\omega}{dk}_{k_0}k_0\right)t}\int dkA\left(k\right)\exp ik\left(x-\left.\frac{d\omega}{dk}\right|_{k_0}t\right)$$

$$= \quad e^{-i\left(\omega_0-\frac{d\omega}{dk}_{k_0}k_0\right)t}\psi\left(x-\left.\frac{d\omega}{dk}\right|_{k_0}t\right)$$

where the last step follows because the integral has the same form as the initial state, $\psi\left(x\right)=\int dkA\left(k\right)\exp ikx$, but with x replaced by $x-\left.\frac{d\omega}{dk}\right|_{k_0}t$. Since the prefactor is just a phase, the probability density moves with velocity $v=v_g=\frac{d\omega}{dk}$,

$$\Psi^*\left(x,t\right)\Psi\left(x,t\right) = \psi^*\left(x-\left.\frac{d\omega}{dk}\right|_{k_0}t\right)\psi\left(x-\left.\frac{d\omega}{dk}\right|_{k_0}t\right)$$

That is the probability distribution remains the same as the initial distribution, moves with velocity $v_{group}=\left.\frac{d\omega}{dk}\right|_{k_0}$.

At time $t=0$, the expectation value of the position of the wave packet is

$$\langle x\rangle=\int dx\psi^*x\psi$$

whereas, at time t it is given by

$$\begin{aligned}\langle x\left(t\right)\rangle &= \int dx\Psi^*x\Psi\\ &= \int dx\psi^*\left(x-v_{group}t\right)x\psi\left(x-v_{group}t\right)\\ &= \int dy\psi^*\left(y\right)\left(y+v_{group}t\right)\psi\left(x-v_{group}t\right)\\ &= \langle x\left(0\right)\rangle+v_{group}t\end{aligned}$$

so the expectation value of the position moves with velocity v_{group}.

2 Schrödinger equation

For the stationary state Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi+V\left(x\right)\psi=E\psi$$

we may take the Fourier transform,

$$\begin{aligned}\psi\left(x\right) &= \frac{1}{\sqrt{2\pi}}\int\limits_{-\infty}^{\infty}A\left(k\right)e^{ikx}dk\\ V\left(x\right) &= \frac{1}{\sqrt{2\pi}}\int\limits_{-\infty}^{\infty}\mathcal{V}\left(k\right)e^{ikx}dk\end{aligned}$$

Then the product $V\psi$ may be written as

$$\begin{aligned}\psi\left(x\right)V\left(x\right) &= \frac{1}{2\pi}\int\limits_{-\infty}^{\infty}\mathcal{V}\left(q\right)e^{iqx}dq\int\limits_{-\infty}^{\infty}A\left(k\right)e^{ikx}dk\\ &= \frac{1}{2\pi}\int\limits_{-\infty}^{\infty}\mathcal{V}\left(q\right)\int\limits_{-\infty}^{\infty}A\left(k\right)e^{i(k+q)x}dqdk\end{aligned}$$

Let $\kappa = k + q$, $\lambda = k - q$

$$\begin{aligned}
\psi(x) V(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathcal{V}(q)\, dq \int_{-\infty}^{\infty} A(k)\, e^{i(k+q)x} dk \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathcal{V}(q)\, dq \int_{-\infty}^{\infty} A(\kappa - q)\, e^{i\kappa x} d\kappa \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathcal{V}(q)\, A(\kappa - q)\, dq \right) e^{i\kappa x} d\kappa
\end{aligned}$$

Then setting the convolution to

$$\left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathcal{V}(q)\, A(\kappa - q)\, dq \right) = \mathcal{B}_{A,V}(k)$$

we cna substitute into the Schrödinger equation,

$$\begin{aligned}
-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \left(\int_{-\infty}^{\infty} A(k)\, e^{ikx} dk \right) + \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathcal{V}(k')\, e^{ik'x} dk' \int_{-\infty}^{\infty} A(k)\, e^{ikx} dk &= E \left(\int_{-\infty}^{\infty} A(k)\, e^{ikx} dk \right) \\
\int_{-\infty}^{\infty} dk e^{ikx} \left(\frac{\hbar^2}{2m} A(k)\, k^2 + \mathcal{B}_{A,V}(k) - E A(k) \right) &= 0
\end{aligned}$$

This is just the Fourier transform of the term in parentheses. Since the Fourier transform is invertible, this term must vanish, and we have

$$E = \frac{\hbar^2}{2m} k^2 + \frac{1}{A(k)} \mathcal{B}_{A,V}(k)$$

This is a dispersion relation for the Schrödinger equation. With $E = \hbar\omega$ we have

$$\omega(k) = \frac{\hbar k^2}{2m} + \frac{1}{\hbar A(k)} \mathcal{B}_{A,V}(k)$$

and the group velocity is

$$\begin{aligned}
v_g &= \frac{d\omega(k)}{dk} \\
&= \frac{\hbar k}{m} + \frac{1}{\hbar} \frac{d}{dk} \left(\frac{\mathcal{B}_{A,V}(k)}{A(k)} \right)
\end{aligned}$$