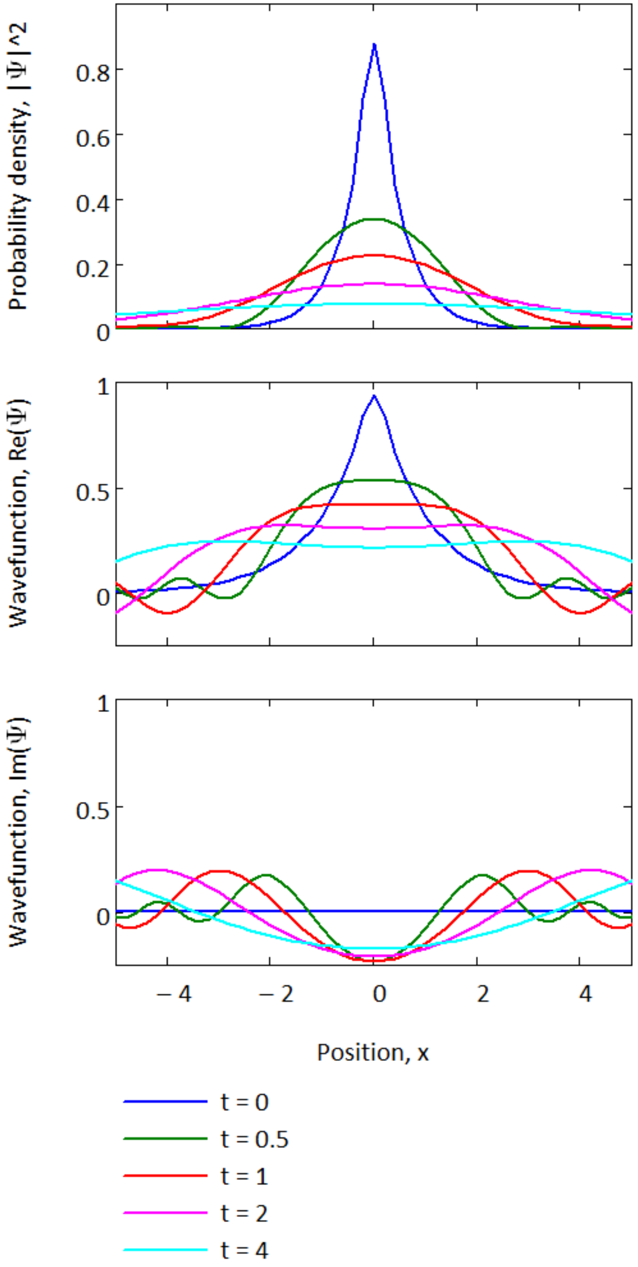
Today in Physics 237: wavepackets

- Free quanta and wavepackets
- Some proofs: Fourier transforms, and proof of the Fourier inversion formula, the free-quantum's version of Fourier's trick
    - Also proof of Parseval's formula/Rayleigh's energy theorem, in which we integrate by completing the square in the exponent, and introduce the Dirac delta function.
- Phase velocity and group velocity in wavepackets



Wavepackets

So the lack of confinement by boundary conditions means that all the stationary solutions $\Psi_k(x,t) = A_k e^{i(kx-\omega t)}$ $= A_k e^{i\left(kx-\hbar k^2 t/2m\right)}$ cannot be normalized and have no definite energy.

- Usually this means that it's an unphysical wavefunction worthy of rejection. But these properties are what we expect and want from a free quantum: it is not confined, and E and $k = \pm\sqrt{2mE}/\hbar$ are **continuous** variables, not quantized.

- So we can still write a general solution; it just has to be an integral this time instead of a sum. And it is normalizable:

$$\Psi(x,t) = \int_{-\infty}^{\infty} A_k e^{i\left(kx-\hbar k^2 t/2m\right)} dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \varphi(k) e^{-i\hbar k^2 t/2m} e^{ikx} dk \quad , \qquad \textbf{Wavepacket}$$

with initial (t = 0) value

$$\boxed{\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \varphi(k) e^{ikx} dk \quad .}$$

- Many (most?) of you will recognize this instantly: the initial, general wavefunction $\Psi(x,t)$ is the **Fourier transform** of the continuous amplitude function $\varphi(k)$.

Wavepackets (continued)

- And those familiar with the Fourier transform are also familiar with **Fourier's inversion formula** – called Plancherel's theorem by G&S – by which the inverse transform is defined:

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

- Both are covered in MATH 281. But because the inversion formula is the continuous-variable, $e^{\pm ikx}$ equivalent of Fourier's trick – very different from the trick used on sines and cosines with quantized arguments – we need to **prove it here**. See also G&S problem 2.19, which is a detailed demonstration.
- First, let $F(k)=\int_{-\infty}^{\infty}f(x)e^{ikx}dx$ and $G(k)=\int_{-\infty}^{\infty}g(x)e^{ikx}dx$. According to **Parseval's formula** (if you're a mathematician) or **Rayleigh's Theorem** (if you're a physicist), which is proven in today's green pages,

$$\boxed{\int_{-\infty}^{\infty}\left|F(k)\right|^2dk=\int_{-\infty}^{\infty}\left|f(x)\right|^2dx\quad ,}$$

Wavepackets (continued)

- Next replace F by $F+G$ and f by $f+g$ in the Rayleigh theorem, and apply the theorem three more times:

$$\int_{-\infty}^{\infty} |F+G|^2\, dk = \int_{-\infty}^{\infty} \left[\overset{2}{\cancel{|F|^2}} + \overset{3}{\cancel{|G|^2}} + 2\mathrm{Re}\left(FG^*\right)\right] dk \overset{\xrightarrow{1}}{=} \int_{-\infty}^{\infty} \left[\overset{2}{\cancel{|f|^2}} + \overset{3}{\cancel{|g|^2}} + 2\mathrm{Re}\left(fg^*\right)\right] dx \quad ;$$

$$\int_{-\infty}^{\infty} \mathrm{Re}\left(FG^*\right) dk = \int_{-\infty}^{\infty} \mathrm{Re}\left(fg^*\right) dx \quad .$$

- Now replace the Rayleigh theorem's F by $F+iG$ and f by $f+ig$, and repeat, using the Rayleigh theorem thrice more. Then add to the previous result:

$$\int_{-\infty}^{\infty} |F+iG|^2\, dk = \int_{-\infty}^{\infty} \left[\cancel{|F|^2} + \cancel{|G|^2} + 2\mathrm{Im}\left(FG^*\right)\right] dk = \int_{-\infty}^{\infty} \left[\cancel{|f|^2} + \cancel{|g|^2} + 2\mathrm{Im}\left(fg^*\right)\right] dx \quad ;$$

$$\int_{-\infty}^{\infty} \mathrm{Im}\left(FG^*\right) dk = \int_{-\infty}^{\infty} \mathrm{Im}\left(fg^*\right) dx \quad \Rightarrow \quad \int_{-\infty}^{\infty} FG^* dk = \int_{-\infty}^{\infty} \left[\mathrm{Re}\left(FG^*\right) + \mathrm{Im}\left(FG^*\right)\right] dk = \int_{-\infty}^{\infty} fg^* dx \quad .$$

Wavepackets (continued)

- Then, let $g(x)=1$ for $0 \le x \le z$, with which $G(k)=\frac{1}{\sqrt{2\pi}}\int_0^z e^{ikx}dx=\frac{1}{\sqrt{2\pi}}\left(\frac{e^{ikz}-1}{ik}\right)$, and use in $\int_{-\infty}^{\infty} FG^* dk=\int_{-\infty}^{\infty} fg^* dx$:

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F\left(\frac{e^{ikz}-1}{ik}\right)^* dk=\int_0^z f dx \quad\Rightarrow\quad \frac{d}{dz}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F\left(\frac{e^{-ikz}-1}{-ik}\right) dk=\frac{d}{dz}\int_0^z f dx \quad\Rightarrow\quad \boxed{\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(k)e^{-ikz} dk=f(z)}$$

, q.e.d.

- The best introductory example to use to illuminate this result is the Gaussian wavepacket, which is the subject of G&S Problem 2.21 (Problem Set #3). This problem can be solved analytically. If you didn't finish it last week, do so before starting problem set #4. Today's green pages will help you.

- Here we'll do an example with a simpler setup, which along with the examples in G&S illuminates why wavepackets seldom have easy analytical solutions.

Problem 2.20. A free quantum has initial wave function $\Psi(x,0)=Ae^{-a|x|}$, where A and a are positive real constants. **a.** Find A. **b.** Find the Fourier amplitudes $\varphi(k)$. **c.** Construct $\Psi(x,t)$, in the form of an integral. **d.** Discuss the limiting cases: *a* very large, and *a* very small.

G&S 2.20

a. Normalize: $1 = A^2 \int_{-\infty}^{\infty} e^{-2a|x|}dx = A^2\left(\int_0^{\infty} e^{-2ax}dx + \int_{-\infty}^{0} e^{2ax}dx\right) = A^2\left(-\frac{e^{-2ax}}{2a}\Big|_0^{\infty} + \frac{e^{-2ax}}{2a}\Big|_{-\infty}^{0}\right) = A^2\frac{1}{a} \Rightarrow \boxed{A = \sqrt{a}}$.

b. Straightforward use of the Fourier inversion formula:

$$\varphi(k) = \sqrt{\frac{a}{2\pi}}\int_{-\infty}^{\infty} e^{-a|x|}e^{-ikx}dx = \sqrt{\frac{a}{2\pi}}\left(\int_0^{\infty} e^{-ax}e^{-ikx}dx + \int_{-\infty}^{0} e^{ax}e^{-ikx}dx\right)$$

$$= \sqrt{\frac{a}{2\pi}}\left(\frac{e^{-(a+ik)x}}{-(a+ik)}\Big|_0^{\infty} + \frac{e^{(a-ik)x}}{a-ik}\Big|_{-\infty}^{0}\right) = \sqrt{\frac{a}{2\pi}}\left(\frac{1}{a+ik} + \frac{1}{a-ik}\right) = \sqrt{\frac{a}{2\pi}}\left(\frac{a-ik}{a^2+k^2} + \frac{a+ik}{a^2+k^2}\right) = \boxed{\sqrt{\frac{a}{2\pi}}\frac{2a}{a^2+k^2}} .$$

c. The time-dependent part is the same as in the stationary solutions, as on page 2. We can't go very far, analytically: the plots on the next page are numerical results.

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\varphi(k)e^{i\left(kx-\hbar k^2t/2m\right)}dk = \boxed{\frac{a^{3/2}}{\pi}\int_{-\infty}^{\infty}\frac{1}{a^2+k^2}e^{i\left(kx-\hbar k^2t/2m\right)}dk} .$$

G&S 2.20 (continued)

d. By large and small we would mean $a \gg |k|$ and $a \ll |k|$ respectively.

Large a: quantum position precisely defined, as $e^{-a|x|}$ is sharply peaked at $x = 0$. Quantum momentum is not, as

$$\varphi(k) = \sqrt{\frac{a}{2\pi}} \frac{2a}{a^2 + k^2} \cong \sqrt{\frac{2}{\pi a}} \left(1 - \frac{k^2}{a^2}\right) \approx \sqrt{\frac{2}{\pi a}}$$

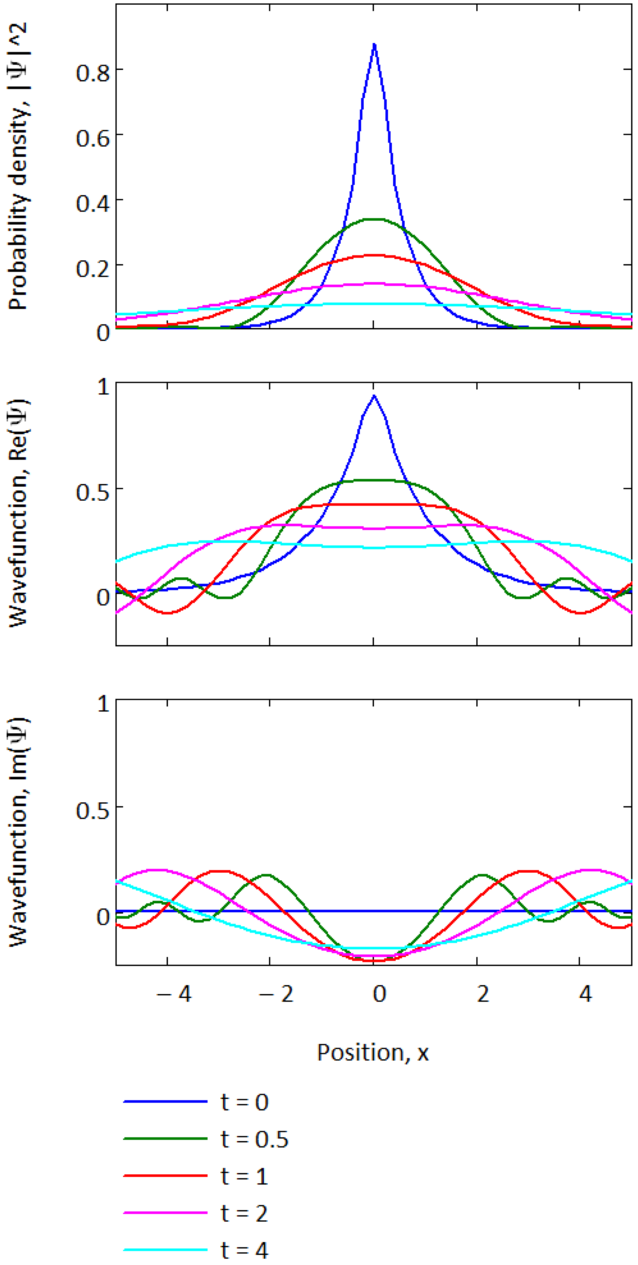
is close to being constant: all values of k about equally represented.

Small a is the reverse:

$$\varphi(k) = \sqrt{\frac{a}{2\pi}} \frac{2a}{a^2 + k^2} \cong \sqrt{\frac{2a^3}{\pi}} \frac{1}{k^2}$$

is sharply peaked at $k = 0$, and $e^{-a|x|} \cong 1 - a|x|$ is close to the same value (1) for a broad range of x.

At right: plots of $|\Psi(x,t)|^2$, $\mathrm{Re}\Psi(x,t)$, and $\mathrm{Im}\Psi(x,t)$.



Phase and group velocity

- Suppose we have a wavepacket resembling the one in Problem 2.20, at small *a* or in the late stages: one with a narrow distribution of *k*, centered at k_0. The difference $s = k - k_0$ is small $\left(s \ll k_0\right)$ for any component of the packed with significant amplitude.

- The same is true for the angular frequency, $\omega = \hbar k^2 / 2m$. We can expand it in a Taylor series about k_0, and keep only the first two terms to good approximation:

$$\omega(k) = \omega_0 + \left.\frac{d\omega}{dk}\right|_{k=k_0}\left(k - k_0\right) = \omega_0 + \omega' s \quad ; \quad \omega_0 = \frac{\hbar k_0^2}{2m}, \quad \omega' = \left.\frac{d\omega}{dk}\right|_{s=0} = \frac{\hbar k_0}{m} \quad .$$

- And use these terms to write the wavepacket's wavefunction:

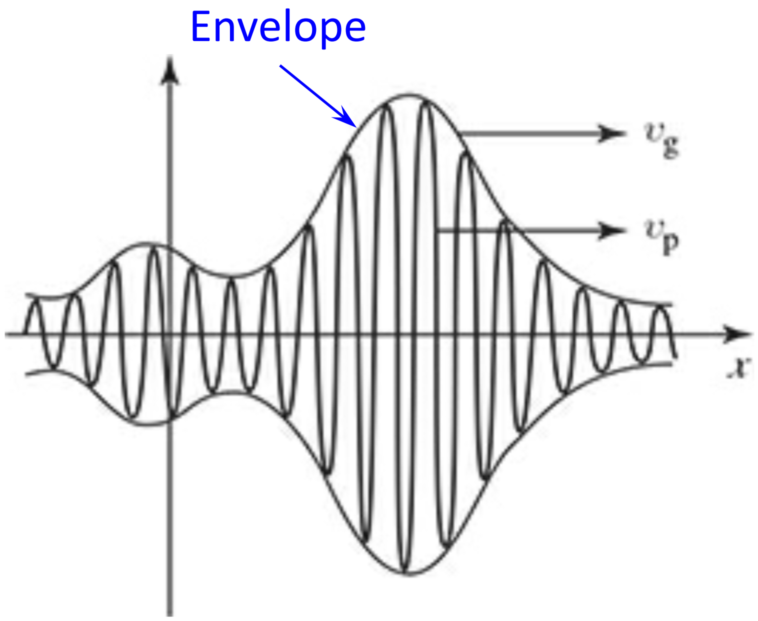
$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\varphi(k)e^{i(kx-\omega t)}dk = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\varphi\left(k_0+s\right)e^{i\left(\left[k_0+s\right]x-\left[\omega_0+\omega'\right]t\right)}ds$$

$$= \frac{1}{\sqrt{2\pi}}e^{i\left(k_0x-\omega_0t\right)}\int_{-\infty}^{\infty}\varphi\left(k_0+s\right)e^{i(sx-\omega' t)}ds \quad ,$$

Phase and group velocity (continued)

where the leading factor is a sinusoidal wave, and the integral which makes up the second factor is the **envelope** of the wavepacket. Both factors travel toward +*x.*

- The sinusoidal wave travels at velocity $v_p = \omega_0 / k_0$. This is the **phase velocity**: the velocity typical of the individual waves which make up the packet.
- The envelope evidently travels at velocity $v_g = \omega' = d\omega / dk\big|_{s=0} = \hbar k_0 / m$. This is the **group velocity**: the velocity that the packet itself travels, meaning the group which carries most of the momentum and energy.
- In Lecture 6 we noted that the velocity of the travelling-wave solution is $v_{\text{quantum}} = \hbar k / 2m = \omega / k$, and that of the corresponding classical particle is twice as large, at $v_{\text{classical}} = \hbar k / m$.
- So the packet's envelope corresponds to the classical particle, as seems highly appropriate.



G&S Figure 2.10

Parseval's formula, a.k.a. Rayleigh's energy theorem

Suppose $F(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{ikx}dx$; then consider the function $I=\int_{-\infty}^{\infty} e^{-\varepsilon^2k^2/2}\left|F(k)\right|^2 dk$. (We will let $\varepsilon\to 0$ at the end.) Expand *I* using the integral expression of *F*, and make a suitable change of dummy-variable name in the second factor of $F(k)F^*(k)$:

$$I=\int_{-\infty}^{\infty} dk\,e^{-\varepsilon^2k^2/2}\left|F(k)\right|^2=\frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,e^{-\varepsilon^2k^2/2}\int_{-\infty}^{\infty} dx\,f(x)e^{ikx}\int_{-\infty}^{\infty} dy\,f^*(y)e^{-iky}$$

$$=\frac{1}{2\pi}\int_{-\infty}^{\infty} dx\,f(x)\int_{-\infty}^{\infty} dy\,f^*(y)\int_{-\infty}^{\infty} dk\,e^{-\varepsilon^2k^2/2+ik(x-y)} \quad .$$

Evaluate the *k* integral by **completing the square in the exponent** (see also G&S Problem 2.19). Abbreviate

$$P=-\frac{\varepsilon^2}{2}k^2+ik(x-y) \quad \text{and} \quad Q=k\sqrt{\frac{\varepsilon^2}{2}}-i(x-y)\sqrt{\frac{1}{2\varepsilon^2}} \quad ; \quad \text{then}$$

Parseval's formula, a.k.a. Rayleigh's energy theorem (continued)

$$Q^2 = \frac{\varepsilon^2 k^2}{2} - \frac{(x-y)^2}{2\varepsilon^2} - 2i\sqrt{\frac{\varepsilon^2}{2}}\sqrt{\frac{1}{2\varepsilon^2}}(x-y)k = -P - \frac{(x-y)^2}{2\varepsilon^2} \quad \Rightarrow \quad P = -Q^2 - \frac{(x-y)^2}{2\varepsilon^2} \quad .$$

The completed square is *Q*'s.

- Substitute this for *P* in the exponent of the *k* integral; note that $e^{-(x-y)^2/2\varepsilon^2}$ comes out of that integral; use $dQ = dk\sqrt{\varepsilon^2/2}$, $-\infty \le \mathrm{Re}\,Q \le \infty$ as $-\infty \le k \le \infty$:

$\sqrt{\pi}$, as per Lecture 2 green pages

$$I = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx\, f(x) \int_{-\infty}^{\infty} dy\, f^*(y) e^{-(x-y)^2/2\varepsilon^2} \frac{\sqrt{2}}{\varepsilon}\int_{-\infty}^{\infty} dQ\, e^{-Q^2} = \frac{1}{\sqrt{2\pi}\,\varepsilon}\int_{-\infty}^{\infty} dx\, f(x) \int_{-\infty}^{\infty} dy\, f^*(y) e^{-(x-y)^2/2\varepsilon^2} \quad .$$

  - **That's this proof's trick:** the original form of *I* has *ε* in the exponent's numerator; now it's in its denominator.

- Switch the order of integration, and substitute $z = y - x,\ dz = dy$:

$$I = \int_{-\infty}^{\infty} dz \frac{e^{-z^2/2\varepsilon^2}}{\sqrt{2\pi}\,\varepsilon}\int_{-\infty}^{\infty} dx\, f(x) f^*(x+z) \quad .$$

Parseval's formula, a.k.a. Rayleigh's energy theorem (continued)

- Observe that first integrand. As $\varepsilon \to 0$, the maximum value of $e^{-z^2/2\varepsilon^2}\Big/\sqrt{2\pi}\,\varepsilon$ increases without bound, and its width (i.e. extent in *z*) narrows to approach zero. But its integral (by itself) doesn't change in the process:

$$\int_{-\infty}^{\infty} dz\,\frac{e^{-z^2/2\varepsilon^2}}{\sqrt{2\pi}\,\varepsilon} = 1 \quad , \quad \text{independent of } \varepsilon.$$

c.f. the Lecture 2 green pages

That matches the definition of the **Dirac delta function:**

$$\boxed{\lim_{\varepsilon\to 0}\frac{e^{-z^2/2\varepsilon^2}}{\sqrt{2\pi}\,\varepsilon} = \delta(z) \quad .}$$

Not to be confused with the Kronecker delta, δ_{mn}.

- So let $\varepsilon \to 0$, and use the fundamental property of the delta function, $\int g(x)\delta(x-a)\,dx = g(a)$ (Lecture 8):

$$\lim_{\varepsilon\to 0} I = \int_{-\infty}^{\infty} dk\,|F(k)|^2 = \int_{-\infty}^{\infty} dz\,\delta(z)\int_{-\infty}^{\infty} dx\,f(x)\,f^*(x+z) \;\Rightarrow\; \boxed{\int_{-\infty}^{\infty} dk\,|F(k)|^2 = \int_{-\infty}^{\infty} dx\,|f(x)|^2} \;.$$

Parseval's formula/
Rayleigh's theorem