The evolution of a wave packet.

Further Properties of Wave Packets

We have seen how [pp. Duality 10-13], by representing a photon as a spatially localized superposition of waves -- i.e. a "wave packet", we can generate the "uncertainty relations" ($\Delta\omega\Delta t \sim 1$, $\Delta k \Delta x \sim 1$) that tell us how closely the photon resembles a <u>wave</u> ($\Delta\omega$ & $\Delta k \to 0$) or a <u>particle</u> (Δt & $\Delta x \to 0$). So wave packets seem to be a promising quantitative representation of the wave-particle duality that we are trying to incorporate into our QM theory. Here we look at some more features of wave packets.

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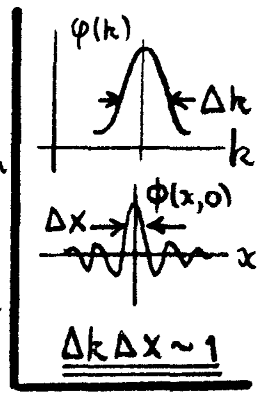
1) Start from a general 1D wave packet, per Eq. (22), p. Duality (22)...

$$\rightarrow \phi(x,t) = \int_{-\infty}^{\infty} \varphi(k)\, e^{i(kx-\omega t)}\, dk. \qquad (1)$$



If the freq. ω and wave # k obey the free-space dispersion relation: $\omega = kc$, then this ϕ represents a photon, as before. However, in general, we can think of $\omega = \omega(k)$ as some more elaborate function of k. We will, however, always think of the spectrum fcn $\varphi(k)$ as being $\sim$ localized in its k-space, so that $\phi(x,0)$ is <u>initially</u> localized to size Δx per: $\Delta k \Delta x \sim 1$. This condition is the essence of a wave packet.

Note that the spectrum fcn $\varphi(k)$ is determined by the initial configuration of ϕ ... at $t=0$ ...

$$\left[\!\left[\ \phi(x,0) = \int_{-\infty}^{\infty} \varphi(k)\, e^{ikx}\, dk \iff \varphi(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \phi(x',0)\, e^{-ikx'}\, dx'. \right.\right. \qquad (2)$$

The integral for $\varphi(k)$ is gotten by a Fourier inverse. This form of $\varphi(k)$, put back into Eq. (1), shows that the packet $\phi(x,t)$ <u>evolves</u> from $\phi(x',0)$ [over all x' @ $t=0$]. The question is: HOW?

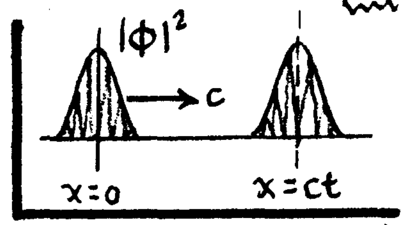
Packet evolution in free space. In a dispersive medium.

The evolution $\phi(x,0) \to \phi(x,t)$ is easy to follow for a free-space photon:

photon in free space : $\omega = kc$,

so// $\phi(x,t) = \int_{-\infty}^{\infty} \varphi(k)\, e^{ik(x-ct)}\, dk = \phi(\xi, 0)$, w/ $\xi = x - ct$. (3)

Thus $|\phi(x,t)|^2$ has same form as $|\phi(\xi,0)|^2$ for



$\xi = x - ct =$ cnst, for a fixed pt. on the packet;

$\Rightarrow$ propagation velocity : $\underline{\underline{v = dx/dt = c}}$, cnst. (4)

The packet moves uniformly to the right @ $v = c$, w/o distortion.

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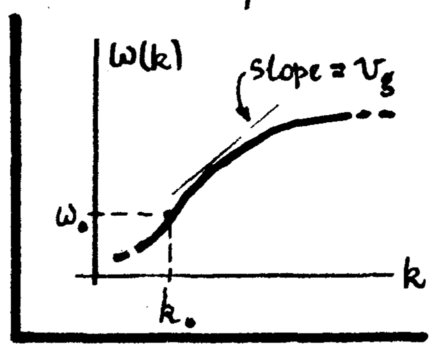
2) The packet evolution is more complicated in a dispersive medium. There : $\lambda\nu = c/n(\lambda)$, $n(\lambda)$ = index of refraction = fcn of wavelength λ. So : $\omega = 2\pi\nu = 2\pi c/\lambda n(\lambda) = \omega(k)$; ω is a general fcn of k...

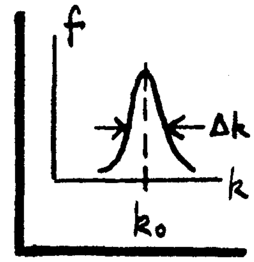
dispersive medium : $\omega = \omega(k)$,

so// $\phi(x,t) = \int_{-\infty}^{\infty} \varphi(k)\, e^{i[kx - \omega(k)t]}\, dk$. (5)



$\phi(x,t)$ is not simply related to $\phi(x,0)$. However, we can get an approximate idea of the evolution by assuming $\phi(x,t)$ is well localized, and $\omega(k)$ does not vary too rapidly with k near the nominal packet wave # k_0...

ϕ localized in Δx $\Big\}$ $\varphi(k) = f(k - k_0)$ $\int$ f is localized in $\Delta k \sim 1/\Delta x$ @ k_0. (6)



Define $\underline{\underline{\kappa = k - k_0}}$ and expand $\omega(k)$ in Taylor series...

$$\omega(k) = \underbrace{\omega(k_0)}_{\omega_0} + (k - k_0)\underbrace{\left[\frac{\partial \omega}{\partial k}\right]_{k=k_0}}_{v_g} + \frac{1}{2}(k-k_0)^2 \underbrace{\left[\frac{\partial^2 \omega}{\partial k^2}\right]_{k=k_0}}_{\alpha} + \cdots$$

i.e.// $\omega(k) = \omega_0 + \kappa v_g + \frac{1}{2}\kappa^2 \alpha + \cdots$, to $\mathcal{O}(\kappa^2)$ w/ $\kappa = k - k_0$. (7)

Packet at early times. Notion of v_g = group velocity.

Here/ ω_0 = nominal packet frequency (there is a spread $\Delta\omega$ about ω_0),
v_g = propagation (group) velocity... see Eq. (10) below,
α = group velocity dispersion... see Eq. ( ) below. (7)

Put the expansion of Eq. (6) into the packet of Eq. (4). Then we can write...

$$\to \phi(x,t) \simeq F(x,t)\exp[i(k_0x-\omega_0 t)] \leftarrow \text{modulated planewave @ } (\omega_0, k_0)$$

$$\text{w/ } F(x,t) = \int_{-\infty}^{\infty} f(\kappa)\, e^{i\kappa(x-v_g t) - \frac{1}{2}i\kappa^2\alpha t}\, d\kappa, \tag{8}$$

$$\text{\&/ } F(x,0) = \int_{-\infty}^{\infty} f(\kappa)\, e^{i\kappa x}\, d\kappa.$$

The main contribution to the integral for $F(x,t)$ comes when $\kappa < \Delta k$, since $f(\kappa)$ is appreciable only in that interval. For short times t, we can make the crude approximation that the term in κ^2 in the exponent in Eq. (7) is ~ negligible:

Assume $t = \Delta t$ is small enough so that : $\underline{\frac{1}{2}\alpha(\Delta k)^2\Delta t \ll 1}$;

$$\text{So/ } F(x,t) \simeq \int_{-\infty}^{\infty} f(\kappa)\, e^{i\kappa(x-v_g t)}\, d\kappa = F(x-v_g t, 0),$$

$$\text{\&/ } |F(x,t)|^2 = |F(\xi,0)|^2, \text{ where: } \xi = x - v_g t. \tag{9}$$

This says that $|\phi(x,t)|^2$ has approximately [at short times] the <u>same</u> <u>shape</u> as the initial value $|\phi(\xi,0)|^2$ for $\xi = x - v_g t$, as in Eq. (3) above. So, have:

$$\to \xi = x - v_g t = \text{cnst} \Rightarrow \text{propagation (group) velocity: } \boxed{v_g = \frac{dx}{dt} = \left(\frac{\partial\omega}{\partial k}\right)_{k_0}}. \tag{10}$$

The packet travels @ $v_g = (\partial\omega/\partial k)_{k_0}$ at early times. This reduces to the free-space result $v_g = c$ [Eq. (4)] when $\omega = kc$ (for photons). Also, this v_g is <u>unique</u> to the expansion in Eq. (7); all the other terms in $(\partial\omega/\partial k)$ vanish when $k = k_0$ (i.e. $\kappa = k - k_0 = 0$).

UNFINISHED BUSINESS
- Ⓐ Is $v_g = (\partial\omega/\partial k)_{k_0}$ consistent with free <u>particle</u> motion?
- Ⓑ What effect does the term in α [in Eq. (7)] have on the motion?

Connection between packet velocity v_g and particle velocity v.

3) Re the "unfinished business" at bottom of last page:

Ⓐ Does $v_g = (\partial\omega/\partial k)_{k_0}$ describe free particle motion?

Should (must) have: $v_g = \partial\omega/\partial k = p/m$ ✓ (p = momentum, m = mass (evaluate @ nominal values)).

But (de Broglie): $p = \hbar k$, so above reads: $\hbar(\partial\omega/\partial p) = p/m$.

Solution to this diff$^{\underline{l}}$ eqtn for ω is: $\omega = p^2/2m\hbar$ (particle freq).

Then (de Broglie): $\underline{\underline{E = \hbar\omega = p^2/2m}}$ ← this is correct particle K.E. (11)

The relations are consistent: a free particle, represented by a wave packet moving @ $v_g = \partial\omega/\partial k$, together with deB's hypothesis, shows the correct classical K.E. Conversely, if we assume free particle motion (and deB), then the particle moves at the wave packet velocity $v_g = \partial\omega/\partial k$.

This packet ↔ particle connection even works relativistically, as follows.

for particle $\begin{cases} E = \gamma mc^2,\ p = \gamma m v, \text{ w/ } \gamma = 1/\sqrt{1-(v/c)^2}; \\ \text{\&/ } E^2 = p^2c^2 + (mc^2)^2 \leftarrow \text{relativistic E-p relation} \end{cases}$

So/ $\begin{pmatrix}\text{differentiate} \\ \text{E-p relation}\end{pmatrix}$ $E\dfrac{\partial E}{\partial p} = c^2 p$, w/ $\underline{\dfrac{\partial E}{\partial p} = c^2\dfrac{p}{E} = v}$ ✓ general velocity for free particle.

Then (de Broglie): $E = \hbar\omega,\ p = \hbar k \Rightarrow \underline{\underline{v = \partial E/\partial p = \partial\omega/\partial k = v_g}}$. (12)

Eqs. (11) & (12) show that identifying a wave packet with a particle gives no big surprises -- at least not for now. The particle's E is consistent with the packet's v_g, assuming nothing more than deB's hypothesis -- which is experimentally verified. The only thing new is deB, and...

→ $\boxed{\text{PARTICLE}}$: $\underline{\underline{\dfrac{\partial E}{\partial p} = v}} \longleftarrow \left(\text{deB}\begin{cases} E = \hbar\omega \\ p = \hbar k \end{cases}\right) \longrightarrow \boxed{\text{PACKET}}$: $\underline{\underline{\dfrac{\partial\omega}{\partial k} = v_g}}$. (13)

This connection is the beginning of a dynamics for our "wavicles."

NOTE in passing... the "dispersion relation" $\omega=\omega(k)$ is quite different for a free particle as compared with a (free) photon...

$$\begin{cases} \text{PHOTONS (free space):} & \omega(k) = kc \leftrightarrow E = pc; \\ \text{PARTICLES (free motion):} & \omega(k) = \hbar k^2/2m \leftrightarrow E = p^2/2m. \end{cases} \tag{14}$$

The dispersion relation $\omega(k)$ is what differentiates one entity from the other; deB's hypothesis: $[E, p] = \hbar[\omega(k), k]$ is deemed universal.

Ⓑ How does $\alpha = \partial^2\omega/\partial k^2$ affect the motion?

In Eq.(9), we neglected α [of Eq.(7)] at short times. We now show that including this term $\Rightarrow$ the packet disperses as time goes on, in accord with the uncertainty relations. In turn, this feature gives a deeper meaning to those relations, but also complicates the interpretation of the wave packet $\phi(x,t)$ as a particle.

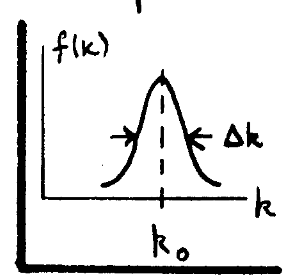
Up through terms of $\mathcal{O}(\kappa^2)$, the form of the packet ϕ is Eq.(8)...

$\rightarrow \phi(x,t) = F(x,t)\exp[i(k_0x - \omega_0 t)]$,

$$\text{w/ } \underline{\underline{F(x,t) = \int_{-\infty}^{\infty} f(\kappa)\exp\{i[\kappa(x-v_g t) - \tfrac{1}{2}\kappa^2\alpha t]\}\,d\kappa}}. \tag{15}$$

NOTE: in what follows re the effects of $\alpha = \partial^2\omega/\partial k^2$, photons are exempt, since for them $\omega(k) = kc$, and $\alpha \equiv 0$.

To see how α enters in, we use an explicit example. Let the spectral fcn $f(\kappa)$ be of a Gaussian form...



$$\begin{cases} f(\kappa) = e^{-\kappa^2/2(\Delta k)^2}, \text{ w/ } \kappa = k - k_0; \\ \text{so } F(x,t) = \int_{-\infty}^{\infty} d\kappa\, e^{-\frac{\kappa^2}{2}\left(\frac{1}{(\Delta k)^2} + i\alpha t\right) + i\kappa(x - v_g t)}. \end{cases} \tag{16}$$

To evaluate this integral, use the tabulated value...

Example of a Gaussian packet : packet diffusion with time.

$$\int_{-\infty}^{\infty} du\, e^{-au^2 \pm bu} = \sqrt{\pi/a}\, \exp(b^2/4a), \text{ for } |a| \neq 0;$$

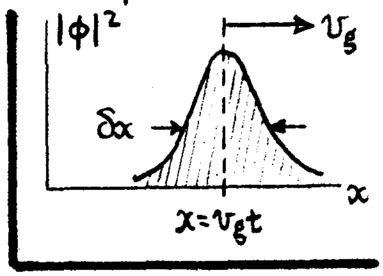
so/ $$F(x,t) = \left[\frac{2\pi(\Delta k)^2}{1+i\alpha(\Delta k)^2 t}\right]^{1/2} \exp\left\{-\frac{(x-v_g t)^2(\Delta k)^2}{2[1+i\alpha(\Delta k^2)t]}\right\}$$ clear imaginary term from denom.

or/ $$F(x,t) = [\quad]^{1/2}\, e^{-\left(\frac{(\Delta k)^2}{2}\cdot\frac{(x-v_g t)^2}{1+[\alpha(\Delta k)^2 t]^2}\right)}\, e^{\frac{i\alpha t}{2}\frac{(\Delta k)^4(x-v_g t)^2}{1+[\alpha(\Delta k)^2 t]^2}}. \tag{17}$$

The intensity of this Gaussian-spectrum wave is then [from Eq. (15)]...

$$\rightarrow |\phi(x,t)|^2 = |F(x,t)|^2 = |[\quad]|\, e^{-(x-v_g t)^2/(\delta x)^2},$$

w/ $$\boxed{\delta x = \frac{1}{\Delta k}\sqrt{1+[\alpha(\Delta k)^2 t]^2}}. \tag{18}$$



The packet intensity $|\phi|^2$ is ~~thus~~ also Gaussian¶ in shape... the packet center moves along @ velocity $v_g = (\partial\omega/\partial k)_{k_0}$, as revealed in Eq. (10) [and even with $\alpha \neq 0$], BUT the packet width δx increases with time t. From Eq. (18), we see that...

$$\begin{cases} \text{initial localization of packet (@ } t=0) \Big\} & \delta x_0 = 1/\Delta k \leftarrow \text{prescription from unc}^{\underline{y}}\text{ rel}^{\underline{n}}\text{s;} \\ \text{localization as } t\to\infty \text{ (i.e. } \alpha(\Delta k)^2 t \gg 1) \Big\} & \delta x \simeq \alpha(\Delta k)t = \alpha t/\delta x_0 \leftarrow \text{packet spreading.} \end{cases} \tag{19}$$

so/ packet diffuses (spreads out) in a characteristic time t_0 such that...

$$\rightarrow \alpha(\Delta k)^2 t_0 \sim 1 \Rightarrow \underline{\underline{t_0 \sim 1/\alpha(\Delta k)^2 = (\delta x_0)^2/\alpha}}, \text{ w/ } \alpha = \left(\frac{\partial^2\omega}{\partial k^2}\right)_0. \tag{20}$$

This is the major effect of α: it destroys the packet localization (and hence its particle-like properties); we cannot maintain $\delta x \sim 1/\Delta k$ @ finite t, so long as $\alpha \neq 0$... as is the case for masses m w/ $\alpha = \partial^2\omega/\partial k^2 = \hbar/m$ [Eq. (14)].

¶ The spectrum fcn $f(k)$ and its Fourier transpose $F(x,0) = \int_{-\infty}^{\infty} f(k)\, e^{ikx} dk$ have the same functional form here (Gaussian). This doesn't happen very often. Another example is : $f(k) = \mathrm{sech}(ka)$. What is the general case?

4) Our fledgling theory is fighting back: the very wave packets ϕ -- which nicely showed particle-like localization (in Δx & Δt) while also maintaining wave-like character (to $\Delta k \sim 1/\Delta x$ & $\Delta\omega \sim 1/\Delta t$) -- now have the property that they <u>disappear</u> in time $t_0 \sim 1/\alpha(\Delta k)^2$, for any "wavicle" with $\alpha = \partial^2\omega/\partial k^2 \neq 0$... as is the case for free particles with $m \neq 0$.*

This development forces the conclusion that -- for a massive particle -- the wave packet intensity $|\phi(x,t)|^2$ <u>cannot</u> represent the spatial distribution of (i.e. the space occupied by) the particle itself... otherwise, the whole universe would just disappear after a sufficient time. Particles must remain localized, and the galloping delocalization of $|\phi(x,t)|^2$ does not reflect this fact. At this point, we have two choices:

(A) Discard wave packets $\phi(x,t)$ as a QM description of matter.

or (B) Interpret $|\phi|^2$ as something other than the particle's spatial location.

What we do now is to try to save ϕ, by choosing (B).

<u>A re-interpretation of ϕ</u> rests on a appeal to the uncertainty relations that characterize all wave packets [ref. p. Duality 12, Eq. (27)]. Consider the spreading packet width δx of Eq. (19). We have...

$$\begin{cases} \text{for free particle: } \omega = \hbar k^2/2m \Rightarrow \alpha = \partial^2\omega/\partial k^2 = \hbar/m, \\ \text{so } \underline{\underline{\delta x \simeq \alpha t/\delta x_0 = \frac{1}{m}(\hbar/\delta x_0)t}}, \text{ w/ } \delta x_0 = \text{initial localization.} \end{cases} \tag{21}$$

Now, by the uncertainty relations, an initial localization to within $\delta x_0 \Rightarrow$ initial momentum uncertainty $\delta p_0 \sim \hbar/\delta x_0$... in 1D, we don't

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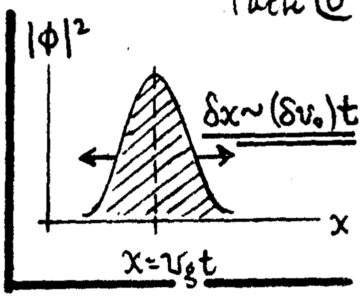
* For photons, with $m = 0 \Rightarrow \omega = kc \Rightarrow \alpha = 0$ (in free space), the "disappearance time" $t_0 \to \infty$. So photons, once born, live forever (in free space).

Packet spreading $\leftrightarrow$ uncertainty relations. Re-interpret ϕ.



know whether the packet expands to the right or left; in 3D, the packet may be expanding in any direction (as well, the packet center is moving at velocity v_g).

The velocity uncertainty $\delta v_0 = \frac{1}{m}\delta p_0 \sim \frac{1}{m}(\hbar/\delta x_0)$ is closely connected with the packet expansion. If we put this δv_0 into Eq. (21), we have...

$\rightarrow$ packet spreading: $\boxed{\delta x \sim (\delta v_0)t}$, δv_0 = velocity uncertainty. (22)

The packet thus follows m's gross motion (@ velocity v_g), and it expands to width δx in just such a way as to cover the possible -- or probable -- extent of m's "wandering" due to the velocity uncertainty δv_0, which was induced by the initial localization to within δx_0. So the uncertainty relation: $(m\,\delta v_0)\,\delta x_0 \sim \hbar$, has a dynamical content, and Eq. (22) is a kind of equation-of-motion for the evolving position uncertainty δx. The packet $\phi(x,t)$ evolves so as to cover all possible locations of m, in accord with this uncertainty relation.

This analysis suggests that we need not interpret $|\phi(x,t)|^2$ as representing the precise location of a massive particle m ($|\phi|^2$ does represent the "precise" location of a photon, with $m=0$)... instead, for $m \neq 0$, we can interpret $|\phi(x,t)|^2$ as the probability of locating m at position x at time t. The uncertainty relation $\Delta p \Delta x \sim \hbar$ has dictated that we really don't "know" where m is at time t, to a precision better than $\delta x \sim (\delta v_0)t$, and $|\phi(x,t)|^2$ -- in its expansion -- reflects this fact. So a QM wave packet description of matter is still possible. BUT, $|\phi|^2$ as a probability of where m has gone, now shares the same "fuzziness" as do the p & x descriptors that obey $\Delta p \Delta x \sim \hbar$.