Stick with wavepackets ϕ as QM descriptors. Need a wave eqtn.

Schrödinger's Wave Equation. The Role of the Wave Function $\psi(\mathbf{r},t)$.

We adopt the point of view that wavepackets are our immediate best chance of dealing with the QM duality that characterizes all matter (photons, electrons, etc.), even though they have some peculiar properties... e.g. they are neither waves (k,ω) nor particles (x,t) to within the uncertainty relations: $\Delta k\,\Delta x \sim 1$ & $\Delta\omega\,\Delta t \sim 1$, and the wavepacket intensity $|\phi|^2$ can at best tell us where a massive "particle" might be, not where it actually is. All this fuzziness is a way-of-life for QM.

We have discovered some important features of how QM wavepackets move by analysing the packet integral: $\phi(x,t)=\int_{-\infty}^{+\infty}\varphi(k)\,e^{i[kx-\omega(k)t]}\,dk$, but we still don't have a wave equation for ϕ... i.e. a PDE like that for the photon: $[\partial^2/\partial x^2 - \frac{1}{c^2}\partial^2/\partial t^2]\,\phi(x,t)=0$, which is not tied down to a particular integral representation. Here we shall derive Schrödinger's wave equation for a massive particle, a PDE for the general ϕ.

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1) Start from a 1D free particle wavepacket...

$$\left.\begin{matrix}\text{dispersion relation for}\\ \text{free particle of mass } m\end{matrix}\right\}\ \omega(k)=\hbar k^2/2m \quad \leftarrow \text{Eq.(14), p. PACK 5.}$$

SO $$\phi(x,t)=\int_{-\infty}^{\infty}\varphi(k)\exp\left[i\left(kx-\frac{\hbar k^2}{2m}t\right)\right]dk \quad \leftarrow \text{free particle wavepacket} \tag{1}$$

This representation of $\phi(x,t)$ depends explicitly on initial conditions, since $\phi(x,t)$ depends on $\varphi(k)$, which is in turn determined by $\phi(x,0)$ [see Eq.(2), p. PACK 1]. Can we get an equation for ϕ that is independent of choosing any particular spectral fcn φ at all? The answer is yes... if we do the following differentiations...

Schrödinger's Wave Eqtn for a Free Particle in 1D. In 3D.

$$\frac{\partial\phi}{\partial t} = -\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\varphi(k)\,k^2 \exp[i(\;)]\,dk;$$

and $$\frac{\partial\phi}{\partial x} = +i\int_{-\infty}^{\infty}\varphi(k)\,k \exp[i(\;)]\,dk,$$

so $$\frac{\partial^2\phi}{\partial x^2} = -\int_{-\infty}^{\infty}\varphi(k)\,k^2 \exp[i(\;)]\,dk = \frac{1}{(i\hbar/2m)}\cdot\frac{\partial\phi}{\partial t};$$

i.e.: $\frac{\partial\phi}{\partial t} = \frac{i\hbar}{2m}\cdot\frac{\partial^2\phi}{\partial x^2}$, or $\boxed{\left(i\hbar\frac{\partial}{\partial t}\right)\phi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\phi}$. SCHRÖDINGER WAVE EQUATION (1D, free particle) (2)

This last relation is Schrödinger's wave eqtn for a free particle of mass m in 1D. The "wave" ϕ does not depend explicitly on initial conditions, as does the Fourier representation of ϕ in Eq. (1).

Generalization of Eq. (2) to 3D is straightforward...

in 3D: $\phi(\mathbf{r},t) = \int_\infty \varphi(\mathbf{k})\exp[i(\mathbf{k}\cdot\mathbf{r}-\omega t)]\,d^3k$ ∫ $\omega = \hbar k^2/2m$, with: $k = |\mathbf{k}|$;

$$\Longrightarrow \underline{\underline{\left(i\hbar\frac{\partial}{\partial t}\right)\phi = \left(-\frac{\hbar^2}{2m}\nabla^2\right)\phi}}, \text{ w/ } \nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2} \;\int \text{Laplace operator} \qquad (3)$$

This result can be obtained by direct differentiation, as in Eq. (2). These results -- either Eq. (2) or Eq. (3) -- are obtained in a wavepacket formalism with just two assumptions: (A) particles & waves are related by the Einstein-de Broglie relations: $(E,p) = \hbar(\omega,k)$, (B) the free particle K.E. is: $E = p^2/2m$.

ASIDE Energy & momentum as operators.

We note that the 1D Schrödinger Eqtn in (2) above could have been "derived" if we had associated operators with E & p as follows...

$$\text{ENERGY: } E \rightarrow \underline{\underline{E_{op}}} = i\hbar\frac{\partial}{\partial t}, \quad \text{MOMENTUM: } p \rightarrow \underline{\underline{p_{op}}} = \frac{\hbar}{i}\cdot\frac{\partial}{\partial x}. \qquad (4)$$

Energy E & momentum p as differential operators.

For then we could have written the self-evident equation...

$$(E)\phi = \left(\frac{1}{2m}p^2\right)\phi \longrightarrow (E_{op})\phi = \left(\frac{1}{2m}p_{op}^2\right)\phi,$$

$$\xrightarrow{\text{by}} \left(i\hbar\frac{\partial}{\partial t}\right)\phi = \frac{1}{2m}\left(\frac{\hbar}{i}\cdot\frac{\partial}{\partial x}\right)^2\phi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\phi \;\checkmark \text{ Same as Eq. (2)} \qquad (5)$$

This maneuver is not as superficial as it looks. For the ϕ in Eq. (1)...

$$E_{op}\phi = \left(i\hbar\frac{\partial}{\partial t}\right)\int_{-\infty}^{\infty}\varphi(k)e^{i(kx-\frac{\hbar k^2}{2m}t)}dk$$

$$= \int_{-\infty}^{\infty}\underbrace{[\hbar^2k^2/2m]}\varphi(k)e^{i(kx-\frac{\hbar k^2}{2m}t)}dk. \qquad (6)$$

this is the particle K.E.: $E = \frac{1}{2m}(\hbar k)^2$, at wave # k.

So $E_{op}\phi$ has the effect of averaging the particle energy E over the extent of the packet. We will say more about E_{op} & p_{op}, later.

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2) We now derive the free particle Schrödinger Eqtn in a different way, to show how it is connected with a photon wave eqtn (and special relativity). Start with the well-known photon wave eqtn from EM...

PHOTONS (in free space)

- Obey 3D wave eqtn: $\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\phi(\mathbf{r},t) = 0$;

  w/ solutions: $\phi(\mathbf{r},t) = \int_{\infty}\varphi(\mathbf{k})e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}d^3k$, $\mathbf{k} = \frac{\omega}{c}\hat{n}$. (propagation direction) (7A)

- Dispersion relation: $k^2 = (\omega/c)^2$ can be obtained from the energy-momentum relation: $(E/c)^2 = p^2 + (mc)^2$, for $m=0$ & $(E,\mathbf{p}) = \hbar(\omega,\mathbf{k})$. (7B)

NOTE: the assumed wavepacket solution for ϕ, plus the dispersion relation $\omega = kc$, is equivalent to the wave eqtn -- you can "derive" the wave eqtn given the integral for ϕ in (7A) and $\omega = kc$ in (7B), in a way similar to Eq. (2) above. To get a wave eqtn for particles, therefore,

Derivation of the Klein-Gordon Eqtn (for a "fat" photon).

we just <u>invert</u> the order of Eqs. (7)...

PARTICLES (moving freely)

- Dispersion relation? Use: $(E/c)^2 = p^2 + (mc)^2$, and: $(E, \mathbf{p}) = \hbar(\omega, \mathbf{k})$, but allow $m \neq 0$. Then, with $k = |\mathbf{k}|$, get...

$$\rightarrow k^2 = (\omega/c)^2 - (mc/\hbar)^2. \qquad (8A)$$

- Wave Eqtn? Assume solutions to desired wave eqtn are <u>packets</u>:

$$\rightarrow \phi(\mathbf{r},t) = \int_\infty \varphi(\mathbf{k})\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\, d^3k\,; \qquad (8B)$$

so// $\nabla^2 \phi(\mathbf{r},t) = -\int_\infty \varphi(\mathbf{k})\, k^2\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\, d^3k,$

and// $\frac{\partial^2}{\partial t^2}\phi(\mathbf{r},t) = -\int_\infty \varphi(\mathbf{k})\, \omega^2\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\, d^3k\,;$

$$\Rightarrow \left[\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]\phi(\mathbf{r},t) = -\int_\infty \varphi(\mathbf{k}) \underbrace{\left[k^2 - \left(\frac{\omega}{c}\right)^2\right]}_{= -(mc/\hbar)^2, \text{ by Eq. (8A)}} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\, d^3k$$

$$= (mc/\hbar)^2 \int_\infty \varphi(\mathbf{k})\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\, d^3k$$

thus// $$\boxed{\left[\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - (mc/\hbar)^2\right]\phi(\mathbf{r},t) = 0}. \qquad (8C)$$

KLEIN-GORDON EQTN
<u>(free particle, mass m)</u>

The Klein-Gordon Eqtn is just the photon wave eqtn of Eq. (7A), but for a "photon" with mass $m \neq 0$. The KG Eqtn is relativistically correct for a zero-spin particle; it includes the photon wave eqtn for the special case of $m = 0$.

We will now show that in the nonrelativistic limit, i.e. $c \to \infty$, the KG Eqtn (8C) reduces to the Schrödinger Eqtn (3). So, Schrödinger's wave eqtn is just the old familiar wave eqtn from Maxwell's EM, but for an old fat photon, moving @ < c, and with $m \neq 0$.

Non Relativistic Limit of the KG Eqtn.

3) To find the nonrelativistic limit of the KG Eqtn (8C), i.e. $c\to\infty$, first look at what happens to the dispersion relation. Note that...

$$\left\{\begin{aligned} E &= mc^2/\sqrt{1-(v/c)^2} \simeq mc^2 + \tfrac{1}{2}mv^2 + \tfrac{3}{8}\left(\tfrac{v}{c}\right)^2 mv^2 + \cdots, \\ \mathbf{p} &= m\mathbf{v}/\sqrt{1-(v/c)^2} \simeq m\mathbf{v} + \tfrac{1}{2}\left(\tfrac{v}{c}\right)^2 m\mathbf{v} + \cdots;\ \text{to } \mathcal{O}\left(\tfrac{v}{c}\right)^2,\ v \ll c. \end{aligned}\right. \tag{9}$$

m is the particle's rest mass, and $\mathbf{v}$ is its velocity. If we neglect the $\mathcal{O}(v/c)^2$ corrections as $c\to 0$, then $\mathbf{p}\simeq m\mathbf{v}$ (Newtonian) and the Einstein relation specifies the KG packet's central frequency ω_0 as...

$$\to \hbar\omega = E = mc^2 + \tfrac{1}{2}mv^2 \simeq mc^2\left[1 + \underbrace{\tfrac{1}{2}(v/c)^2}_{\text{neglect, as } c\to\infty}\right]$$

So// $\underline{\omega \simeq mc^2/\hbar = \omega_0}$, in NR limit. (10)

This (large) freq. formally $\to\infty$ as $c\to\infty$, and we don't want it appearing in the KG Eqtn, as it does in Eq. (8C). We can factor ω_0 out of the problem by defining a new version ψ of the KG packet ϕ, viz.

$$\left\{\begin{aligned} &\text{Let}: \psi(\mathbf{r},t) = e^{i\omega_0 t}\phi(\mathbf{r},t); \\ &\text{so}//\ \nabla^2\phi = e^{-i\omega_0 t}\nabla^2\psi, \\ &\text{and}//\ \frac{\partial^2}{\partial t^2}\phi = e^{-i\omega_0 t}\left[\frac{\partial^2}{\partial t^2} - \overbrace{\left(\frac{2i\omega_0}{c^2}\right)}^{\omega_0/c^2 = m/\hbar}\frac{\partial}{\partial t} - \overbrace{\left(\frac{\omega_0}{c}\right)^2}^{\omega_0/c = mc/\hbar}\right]\psi. \end{aligned}\right. \tag{11}$$

Evidently ψ & ϕ differ only by a phase factor ($e^{i\omega_0 t}$), and they specify equivalent QM position probabilities, because $|\psi|^2 \equiv |\phi|^2$. By the $\phi\to\psi$ transform here, the KG Eqtn: $\left[\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]\phi = (mc/\hbar)^2\phi$, in Eq. (8C), is transformed -- after minor algebra -- to...

$$\boxed{\nabla^2\psi + (2im/\hbar)\frac{\partial}{\partial t}\psi = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi} \tag{12}$$

TRANSFORMED KG EQTN
($\psi = \phi e^{i\omega_0 t}$, free particle)

This eqtn is still exact, but now it is easy to see how to take the NR limit $c\to\infty$. In that case, the RHS term becomes negligibly small, and we have:

Schrödinger Eqtn regained (for a fat, slow photon). $|\psi|^2$ interpretation.

$$\nabla^2\psi + (2im/\hbar)\frac{\partial}{\partial t}\psi \rightarrow 0, \text{ as } c\rightarrow\infty;$$

i.e. $$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi = i\hbar\frac{\partial}{\partial t}\psi}$$ SCHRÖDINGER WAVE EQTN (as NR limit of KG Eqtn) (13)

So we are back to the Schrödinger Eqtn, same as Eq(3) above. Indeed, Schrödinger's Eqtn is just a "standard" wave eqtn for a fat photon ($m \neq 0$) that is not moving very fast ($v \ll c$). In that sense, it is not new. What is new is the interpretations that are attached to the roles of the dynamical variables in the problem [QM duality demands: $(E, \mathbf{p}) = \hbar(\omega, \mathbf{k})$, and a packet description implies uncertainties: $\Delta E\Delta t \sim \hbar$, $\Delta p\Delta x \sim \hbar$], and to the role of the wave function ψ itself [$|\psi|^2$ does not measure the actual presence of the particle, but only the probability of its presence].

NOTE: at this point, we will call the ψ in Schrödinger's Eqtn, Eq.(13), a "wave function" for particle m, rather than a "packet amplitude". This nomenclature follows common usage.

UNFINISHED BUSINESS
- Ⓐ Can $|\psi|^2$ really be interpreted as a probability distribution?
- Ⓑ How is Eq.(13) modified by the presence of external forces?

We can deal fairly quickly with point Ⓐ; point Ⓑ requires elaboration.

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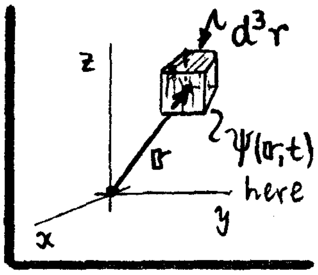
4) Re point Ⓐ: is the interpretation of $|\psi|^2 \propto$ probability of finding m at a particular location consistent with the wave eqtn [Eq.(13)] itself? In this interpretation [see remarks on p. Pack 8], we claim...

$\rightarrow |\psi(\mathbf{r},t)|^2 \propto$ probability of finding m at position $\mathbf{r}$ at time t. (14A)

But the probability of finding m at or near $\mathbf{r}$ must also depend on the size of the volume element d^3r that we sample in that neighborhood.

Schrödinger's $|\psi|^2$ as a probability density.

So we incorporate this volume factor, and we define:



$$|\psi(\mathbf{r},t)|^2 d^3r = \text{probability of finding } m \text{ in volume element } d^3r \text{ at position } \mathbf{r} \text{ at time } t. \quad (14B)$$

In order for this to work, i.e. in order that $|\psi|^2$ be an acceptable probability density, we need to impose a restriction on its "size", viz.

① $\int_\infty |\psi(\mathbf{r},t)|^2 d^3r = \text{cnst.}$ $\int_\infty \Rightarrow$ integration over all space. The "cnst" can be chosen $\equiv 1$ (normalization)* (15A)

This is the statement that m, if it exists, must be found somewhere in the space. Eq. (15A) is required for conservation of particles.

② Not only should $\int_\infty |\psi|^2 d^3r = \text{cnst}$ when integrated over all space, but this cnst must be time-independent (otherwise m may disappear after awhile). So:

$$\frac{\partial}{\partial t}\int_\infty |\psi(\mathbf{r},t)|^2 d^3r = 0, \text{ for particles conserved in time.} \quad (15B)$$

We will now show that conditions (15A) & (15B) are automatically satisfied for any "reasonable" ψ that satisfies Schrödinger's free particle eqtn, Eq. (13).

We have, for the time-rate-of-change of the (proposed) probability $\mathcal{P}$...

$$\dot{\mathcal{P}} = \frac{\partial}{\partial t}\int_\infty |\psi|^2 d^3r = \int_\infty \left[\frac{\partial}{\partial t}(\psi^*\psi)\right] d^3r, \quad \left(\begin{array}{c}\text{the * denotes}\\ \text{complex conjugate}\end{array}\right)$$

or,

$$\dot{\mathcal{P}} = \int_\infty (\partial\psi^*/\partial t)\,\psi\, d^3r + \int_\infty \psi^*(\partial\psi/\partial t)\, d^3r. \quad (16A)$$

But, by Schrödinger's Eqtn: $\frac{\partial\psi}{\partial t} = (i\hbar/2m)\nabla^2\psi$, and: $\frac{\partial\psi^*}{\partial t} = -(i\hbar/2m)\nabla^2\psi^*$.

By putting these expressions into Eq. (16A), we obtain...

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* The Schrödinger Eqtn: $\partial\psi/\partial t = (i\hbar/2m)\nabla^2\psi$, is linear in ψ. Then, if ψ is a solution, so is $\mathcal{N}\psi$ -- where $\mathcal{N}$ is any cnst independent of $\mathbf{r}$ & t. $\mathcal{N}$ is called a "normalization cnst", and it can be adjusted to meet the requirement in (15A) that: $\int_\infty |\psi|^2 d^3r = 1$. Then, evidently, $\mathcal{N}$ has dimensions of $1/\sqrt{\text{volume}}$.

Conservation of particles for $|\psi(\text{Schrödinger})|^2$.

$$\rightarrow \dot{\mathcal{P}} = (i\hbar/2m)\int_\infty \underbrace{[\psi^*(\nabla^2\psi) - (\nabla^2\psi^*)\psi]}\, d^3r \qquad \text{(16B)}$$

... use Green's Identity : $[\;] = \nabla\cdot[\psi^*(\nabla\psi) - (\nabla\psi^*)\psi]$...

$$\text{So/} \quad \dot{\mathcal{P}} = (i\hbar/2m)\int_\infty \nabla\cdot[\psi^*(\nabla\psi) - (\nabla\psi^*)\psi]\, d^3r \qquad \text{(16C)}$$

... use Gauss' Divergence Thm : $\int_\infty \nabla\cdot\mathbb{A}\, d^3r = \oint_\infty \mathbb{A}\cdot d\mathbb{S}$ ...

$$\text{So/} \quad \dot{\mathcal{P}} = (i\hbar/2m)\oint_\infty [\psi^*(\nabla\psi) - (\nabla\psi^*)\psi]\cdot d\mathbb{S} \qquad \text{(16D)}$$

$\int$ $\mathbb{S}$ is a closed surface which has receded to ∞.

... use $(z - z^*) = 2i\,\mathrm{Im}\,z$, for z = complex # ...

$$\text{So/} \quad \underline{\dot{\mathcal{P}} = \frac{\partial}{\partial t}\int_\infty |\psi|^2 d^3r = (\hbar/m)\,\mathrm{Im}\oint_\infty [\psi(\nabla\psi^*)]\cdot d\mathbb{S}}. \qquad \text{(16E)}$$

$\dot{\mathcal{P}}$ is not apparently zero, as required by Eq. (15B). BUT, if we claim that the wavefcn ψ we are dealing with is a localized packet, then we say...

localized packet $\}$ ψ & $\nabla\psi \rightarrow 0$, on the surface $\mathbb{S}$ at ∞,

So/ $\underline{\dot{\mathcal{P}} = (\hbar/m)\oint_\infty [\psi(\nabla\psi^*)]\cdot d\mathbb{S} \rightarrow 0}$, localized particles conserved. (16F)

Localization of ψ is (almost) always the case*, and for such ψ's we have shown that particles are conserved : $(\partial/\partial t)\int_\infty |\psi|^2 d^3r = 0$, as required by Eq. (15B). Note that (15A) follows then by a simple time integration. So...

$$\boxed{\text{Schrödinger's Eqtn itself, plus localization of } \psi \Rightarrow \text{particle conservation.}} \qquad \text{(17)}$$

Had this not worked, we would be forced to junk the notion of interpreting $|\psi|^2$ as a probability distribution. But... so far, so good...

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* An exception are free particle planewaves : $\psi_k(\mathbf{r},t) = \mathcal{N}e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}$, for an m with momentum $\hbar k$ and energy $\hbar\omega = \frac{1}{2m}(\hbar k)^2$. These ψ_k's satisfy Schrödinger's Eqtn, with $|\psi_k|^2 = |\mathcal{N}|^2$ = cnst everywhere. Clearly $|\psi_k|^2$ is not localized, and does not vanish at ∞. We will deal with this exceptional case later.