## Expanded Comments on Wave Packets

**Comments on Section 7.2, page 160.**

In classical mechanics, one talks about particles that have position $x$ and velocity $v$. In quantum mechanics, one is no longer allowed to speak that way. Particles are replaced by waves, and position and velocity cannot be specified simultaneously. Still, there must be something one can describe in quantum mechanics that acts like a particle. There must be some way to describe things that move through space with definite positions and velocity, and some way to understand the limits quantum mechanics places on viewing them that way.

Here is a first guess. Write down a wave function that is a delta function centered at position $r_0$. Take that to be a particle. Disaster! It doesn't act like a particle at all. It spreads out to both sides, and there is no way to make it move at a desired velocity. Of course, if one wants something with definite velocity, one can write down a wave function $\exp[imv.r/\hbar]$, but this is a disaster too, since it has no definite location. So what one needs is a function that has a definite wavelength like a plane wave, and a definite position like a delta function. Well, there is no way to have both at the same time, but one can aim for a compromise.

The compromise is called a wave packet. There are two ways to build them. First: Suppose one has a bunch of solutions to Schrodinger's equation of the sort that come from Bloch's equation:

$$\psi_k(r) \tag{1}$$

These have a definite momentum, but are not localized in space. Next suppose that $F(r-r')$ is a function that has a peak when $r=r'$, and drops to zero on either side. If the distance scale where $F$ drops to zero is much larger than the period of $\psi$, then

$$\psi_k(r)F(r-r') \tag{2}$$

is a wave packet centered at $r=r'$, and with wavenumber $k$. Now this is all very nice, and a wave shaped like this would have properties like a particle as it should, but unfortunately I don't know of any good way to show that. To make some progress with a wave packet analytically, it is necessary to move to the second way of forming them.

The second way is based upon the identity

$$\int \frac{dk}{2\pi}e^{ikr} = \delta(r) \tag{3}$$

What this identity suggests is that if one adds together lots of extended waves of different wave numbers, they should form something that is localized in space. So, form the sum

$$W(r,k) = \sum_{k'} w(k-k')\psi_{k'}(r) \tag{4}$$

Here $w(k-k')$ is a dimensionless function that has a peak at $k=k'$, and drops to zero on either side. It should drop to zero slowly compared to the scale where $\psi_k'$ varies as a function of $k'$. This sum should be expected to produce a wiggly function with a peak at $r=0$, and with a wiggle whose wave number is approximately $k$. The big difference between this prescription for a wave packet and the previous one is that now one knows how the packet evolves in time. The first definition involved the product of two functions of space. If one puts it into Schrodinger's equation, there is absolutely nothing one can say

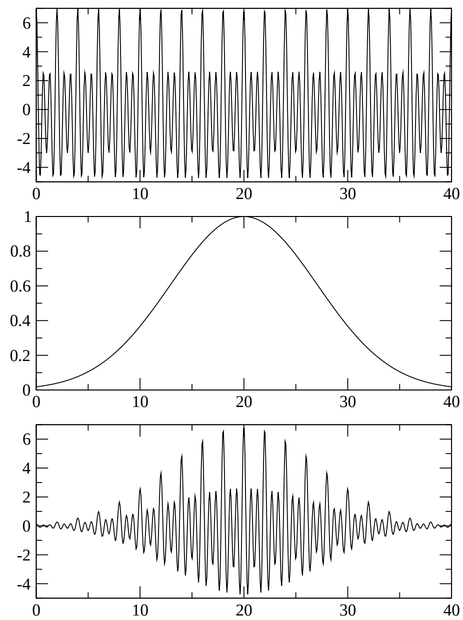


**Figure 1**. A wave packet can be constructed by multiplying a wave by a modulating function that makes the wave die off to the right and to the left.

about what it will do. However, the second definition is simply a sum of spatial functions, and its time evolution is simply

$$W(r, k, t) = \sum_{k'} w(k-k')\psi_{k'}(r)e^{-i\mathcal{E}_{k'}t/\hbar}. \tag{5}$$

At this point, I have almost recovered Equation (7.26). But actually, in going through this argument I have decided that (7.26) is not quite right! I would prefer it to read

$$W(r, k, t) = \int [d\vec{k}']\; w(k-k')e^{ik'r-i\mathcal{E}_{k'}t/\hbar}\left[\psi_{k'}(r)e^{-i\vec{k}'\cdot\vec{r}}\right] \tag{6}$$

$$\approx e^{i\vec{k}\cdot\vec{r}-i\mathcal{E}_{\vec{k}}t/\hbar}\int [d\vec{k}'']\; w(\vec{k}'')\; e^{-i\vec{k}''\cdot(\vec{r}-\vec{\nabla}_{\vec{k}}\mathcal{E}_{\vec{k}}t/\hbar)}\left[\psi_{\vec{k}}(\vec{r})e^{-i\vec{k}\cdot\vec{r}}\right], \tag{7}$$

Defining $\vec{k}'' = \vec{k} - \vec{k}'$ and expanding the terms in the exponent to first order in $\vec{k}''$, because $w$ is peaked about $\vec{k}'' = 0$.

$$\approx e^{i\vec{k}\cdot\vec{r}-i\mathcal{E}_{\vec{k}}t/\hbar}\;\mathcal{F}\;(\vec{r}-\vec{\nabla}_{\vec{k}}\mathcal{E}_{\vec{k}}t/\hbar) \tag{8}$$

The value of the integral $\mathcal{F}$ does not matter; just the fact that it is in the form of a traveling wave moving at $\vec{v}_{\vec{k}} = \vec{\nabla}_{\vec{k}}\mathcal{E}_{\vec{k}}/\hbar$.

In the last term I simply drop $[\psi_k(r)e^{-ikr}]$ on the grounds that if $\psi_k$ is enough like a plane wave, then this term will be constant. Of course, that argument is neither satisfying, nor completely right, which explains why in the more careful analysis in Chapter 16, some extra terms appear.

Some final comments to complete the argument: $\mathcal{F}(\vec{r} - \vec{\nabla}_{\vec{k}}\mathcal{E}_{\vec{k}})$ describes a traveling wave moving at velocity

$$\vec{v} = \vec{\nabla}_{\vec{k}}\mathcal{E}_{\vec{k}}/\hbar. \tag{9}$$

Identifying $\omega = \mathcal{E}_{\vec{k}}/\hbar$ gives the familiar group velocity

$$\vec{v} = \frac{\partial\omega}{\partial\vec{k}}. \tag{10}$$

### 0.0.1 Comments on section 16.4.1, page 426

The formalism in Section 16.4 clears up all the uncertainties from Chapter 7. At least, that is the main thing it is intended to do. But simultaneously the section produces a certain sense of shock and surprise because the simple and comforting relation $v = \partial\omega/\partial k$ has transformed itself into something complicated, with a long formal derivation, and extra unfamiliar terms at the end..

First a few words on why I wrote the section the way I did. If one wants a nice heuristic derivation of wave packet motion, then the treatment on page 160, or in section 16.2.2, or in Problems 16.7 and 16.9 will do. The difficulty with the various heuristic derivations is that they all get the wrong answer. They miss some terms. Now the fact that these terms are generally unknown and omitted has not greatly hampered the progress of physics. There are many cases where they vanish, and they do not enter the electron transport equations that are most commonly used. However, it seemed to me that with experiments becoming every more precise and exploring ever smaller spatial scales, it is just a matter of time before the effect of these terms on electron motion needs to become part of general knowledge. So I decided to include a derivation of the correct semi-classical electron equations of motion. It is not very long, but it is fairly heavy going, and relies on the Lagrangian formalism in Appendix B.3, which is very simple, but also generally unfamiliar.

Next, a bit of a discussion of Eq. (16.65). This drops a bit out of the blue, but after the remarks above in these notes it may no longer seem so mysterious. Once again, one supposes that solutions of Schrödinger's equation are known. These are solutions when electric and magnetic field are both zero. Now build a wave packet. Similar to Eq. (4), take

$$W_{\vec{k}_c}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_{\vec{k}} w_{\vec{k}\vec{k}_c}\psi_{\vec{k}}(\vec{r}). \tag{11}$$

If $\psi$ is something like a plane wave, the result at this point should be a wave packet peaked near zero. Suppose I want a wave packet centered somewhere else, say at $r_c$? Well, if $\psi$ is something like a plane wave $e^{i\vec{k}\cdot\vec{r}}$, then I can offset it through multiplying by $e^{-i\vec{k}\cdot\vec{r}_c}$. So now I guess

$$W_{\vec{r}_c\vec{k}_c}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_{\vec{k}} w_{\vec{k}\vec{k}_c}e^{-i\vec{k}\cdot\vec{r}_c}\psi_{\vec{k}}(\vec{r}). \tag{12}$$

This is getting close to a good starting guess for the wave packet. There is no simple way to see that it is not quite good enough. Sometimes derivations are a bit like trips through a maze, where one has to travel a fairly long distance to see whether or not they are dead ends. In this case, if one used Eq. (12), one would hit a dead end a long time later in the derivation, if a magnetic field were present. The problems would arise on page 428 in trying to pass from Eqs. (16.79) and (16.80) to Eq. (16.82). Notice that the electric and magnetic fields enter in different ways. The electric field enters through $-eV(\vec{r})$. If the electric field is constant, this is simply $e\vec{E}\cdot\vec{r}$. Because of Eq. (16.78), the expectation value of the electric potential inside a wave packet is rigorously $e\vec{E}\cdot\vec{r}_c$.

The magnetic field enters differently, through terms involving the square of the vector potential. One will have to evaluate a term involving $r^2$ such as

$$\langle W_{\vec{r}_c\vec{k}_c}|\frac{B^2}{2}r^2|W_{\vec{r}_c\vec{k}_c}\rangle \tag{13}$$

Unfortunately there is no formal result for $r^2$ that matches the certainty provided by Eq. (16.78). The safest thing to do is to make this term as small as possible, and then argue that it can be neglected if $B$ is not too large. This goal would be accomplished if instead of Eq. (13) one had

$$\langle W_{\vec{r}_c\vec{k}_c}|\frac{B^2}{2}(r-r_c)^2|W_{\vec{r}_c\vec{k}_c}\rangle. \tag{14}$$

Since $W_{\vec{r}_c\vec{k}_c}$ is a localized wave packet centered at $r_c$, it is easy to believe that Eq. (14) would be much smaller than Eq. (13), and that one could justify throwing it away. So, turning back to the beginning, define the wave packet to be

$$W_{\vec{r}_c\vec{k}_c}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_{\vec{k}} w_{\vec{k}\vec{k}_c} e^{-ie\vec{A}(\vec{r}_c)\cdot\vec{r}/\hbar c - i\vec{k}\cdot\vec{r}_c}\psi_{\vec{k}}(\vec{r}). \tag{15}$$

The extra phase factor involving the magnetic potential lies dormant on pages 426 and 427, but on page 428 it springs into action. It has the effect of replacing Eq. (16.80) by

$$\hat{\mathcal{H}} = \frac{1}{2m}\left[\hat{P} + \frac{e\left[\vec{A}(\vec{r}) - \vec{A}(\vec{r}_c)\right]}{c}\right]^2 + U(\vec{r}). \tag{16}$$

So by introducing just the right set of wiggles in the original wave packet, one can center it where desired, and make the world safe later for approximations involving the magnetic field.

Most of the calculations on pages 426–428 are, as they say, tedious but straightforward, and most of the details are in problems. Some things could have been done in different ways.

For example, Eq. (16.78) is a really basic property of wave packets, and one will do whatever it takes to make it true. So it might be better to begin page 427 by demanding that Eq. (16.78) hold, and then working backwards until one arrives at Eq. (16.69), which is the condition on the phase of $w$ that makes it all work.

I should have referred to Appendix B.3 on page 428 rather than assuming that one remembers its existence from top of page 426.

Finally, worked solutions to all problems are available in the instructor's manual, which means that instructors can get written copies of gory details for page 428 just by asking me for them.