Math 676 (Olivier) Class Notes

Colin Roberts

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1 Physics Prerequisites

1.1 Waves

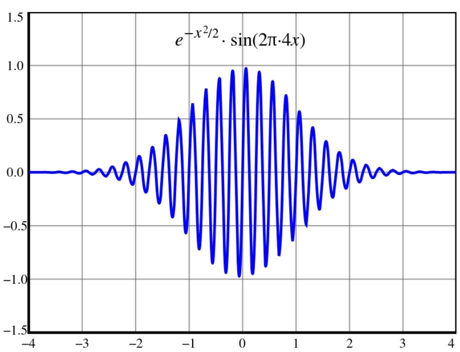
We describe the electromagnetic field via $(\vec{E}(t,x), \vec{B}(t,x))$ with $\vec{E}$ representing the electric field and $\vec{B}$ representing the magnetic field. Of course, t represents time and x represents position (x could potentially be a vector in $\mathbb{R}^3$).

- Suppose we have a wave that is described by a scalar field $\phi(t,x)$, which is a solution to the wave equation
$$\partial_t^2\phi - c^2\Delta\phi = 0.$$
Then we say the intensity is $I(t,x) = |\phi(t,x)|^2$. We denote $\phi(0,x)$ by $\phi_0(x)$.

- Equivalently, we could choose to represent this solution in Fourier space by transforming from spatial coordinates x to wave vector coordinates k. We then have
$$\phi(t,x) = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\hat{\phi}_0(k)e^{i(kx-\omega t)}dx.$$
By Fourier-Plancherel we then have that
$$\int_{\mathbb{R}^3}|\phi(t,x)|^2dx = \int_{\mathbb{R}^3}|\hat{\phi}_0(k)|^2dk.$$
It then follows that in Fourier space, we have
$$-\omega^2 + c^2|k|^2 = 0$$
iff ϕ is a solution to the wave equation. In other words, ϕ satisfies the *dispersion relation* $\omega^2 = c^2|k|^2$.

- $\hat{\phi}_0(k)$ is smooth and has compact support. Meaning that $\hat{\phi}_0(k) = 0$ for $|k| \geq K$ for some positive K.

- We see that $\phi(t,x)$ has the following form:



- Finally we have that $\hat{\phi}(t,k) = \hat{\phi}_0(k)e^{i(kx-\omega t)}$ as the time-evolved state.

1.2 Position and Momentum Operators

We will use the following notation for the inner product $(u,v) = \int_{\mathbb{R}^3} \overline{u}(x)v(x)dx$ and for the norm $\|u\|^2 = (u,u)$.

Definition 1.1. The *average position of a wave packet* is

$$\langle x(t) \rangle := \frac{\int_{\mathbb{R}^3} x|\phi(t,x)|^2 dx}{\|\phi(t,\cdot)\|^2}.$$

The *momentum* is then $\vec{p} = \hbar\vec{k}$. Then the *average value of the momentum for the wave packet* is given by

$$\langle p(t) \rangle := \frac{\int_{\mathbb{R}^3} \hbar k|\hat{\phi}(t,k)|^2 dk}{\|\hat{\phi}(t,\cdot)\|^2}.$$

From here on out we restrict to normalized states, i.e., $\|\phi(t,\cdot)\| = 1$.

Definition 1.2. The *position operator* $X_i\varphi = x_i\varphi$ for $i = 1,2,3$. Note that for $\phi \in L^2(\mathbb{R}^3)$ we may not have that $X_i \colon L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$.

Definition 1.3. The momentum operator is $P_j\varphi(x) = i\hbar\frac{\partial}{\partial x_j}\varphi(x)$ for $j = 1,2,3$.

Remark. Of course we can Fourier transform the above operators. The Fourier transform of the position operator becomes differentiation with respect to k and the Fourier transform of the momentum operator becomes multiplication by $\hbar k$.

It follows that we can write the expected values for the position and momentum in the following way:

$$\begin{aligned}
\langle X_j \rangle &= (X_j\phi(t,\cdot), \phi(t,\cdot)), \\
\langle P_j \rangle &= (P_j\phi(t,\cdot), \phi(t,\cdot)).
\end{aligned}$$

Proposition 1. *X_j and P_j are symmetric operators. Meaning that for smooth functions ϕ, ψ we have that*

$$\begin{aligned}
(X_j\phi, \psi) &= (\phi, X_j\psi), \\
(P_j\phi, \psi) &= (\phi, P_j, \psi).
\end{aligned}$$

Moreover, X_j and P_j satisfy the Heisenberg commutation relations:

$$\begin{aligned}
X_iP_j &= P_jX_i, && i \neq j \\
P_iX_i - X_iP_i &= -i\hbar\mathbf{I}.
\end{aligned}$$

Proof. Left as an exercise. *Hint:* $P_i(X_i\varphi) - X_i(P_i\varphi) = -i\hbar\varphi$. ☐

Since we were able to find the center of the wave packet, $\langle X_i \rangle$ (for position, at least). We wish to find the width of the wave packet in order to fully characterize the state. We have that the width is

$$\begin{aligned}
(\Delta X_j)^2 &= \int_{\mathbb{R}^3} |x_j - \langle X_j \rangle|^2 |\phi(t,x)|^2 dx \\
&= \|x_j\phi(t,\cdot\|^2 - (\langle X_j \rangle)^2.
\end{aligned}$$

Proposition 2. *Let A, B be symmetric operators that satisfy Heisenberg's commutation relation $AB - BA = i\hbar\mathbf{I}$, then*

$$\|A\varphi\|^2\|B\varphi\|^2 \geq \frac{\hbar^2}{4}\|\varphi\|^4.$$

Proof. Let $\lambda \in \mathbb{R}$. So then $\|(A+i\lambda B)\varphi)\|^2 = \|A\varphi\|^2 + 2\text{Re}(A\varphi, i\lambda B\varphi) + \lambda^2\|B\varphi\|^2$. Now we have

$$\begin{aligned}
\text{Re}(A\varphi, i\lambda B\varphi) &= -\lambda \text{Im}(A\varphi, B\varphi) \\
&= -\lambda \text{Im}(\varphi, AB\varphi) && \text{since } A, B \text{ is symmetric} \\
&= -\lambda \text{Im}(BA\varphi, \varphi) \\
&= -\lambda \text{Im} \int_{\mathbb{R}^3} \overline{BA\varphi}\varphi dx \\
&= \lambda \text{Im} \int_{\mathbb{R}^3} \overline{\varphi} BA\varphi dx.
\end{aligned}$$

So now,

$$\begin{aligned}
2\text{Re}(A\varphi, i\lambda B\varphi) &= -\lambda \text{Im}(\varphi, (AB - BA)\varphi) \\
&= -\lambda \text{Im}(i\hbar \|varphi\|^2) \\
&= -\lambda\hbar\|\varphi\|^2.
\end{aligned}$$

So,

$$\begin{aligned}
\|A\varphi\|^2 - \lambda\hbar\|\varphi\|^2 - \lambda^2\|B\varphi\|^2 &\geq 0 && \forall \lambda \in \mathbb{R} \\
\implies \hbar^2\|\varphi\|^4 &\leq 4\|B\varphi\|^2\|A\varphi\|^2 && \text{using a discrimant or something} \\
\implies \|B\varphi\|\|A\varphi\|^2 &\geq \frac{\hbar}{2}\|\varphi\|^2.
\end{aligned}$$

□

Theorem 1.1. *Define* $\Delta X_i = \sqrt{\|X_i\phi\|^2 - \langle X_i \rangle^2}$, $\Delta P_i = \sqrt{\|P_i\hat{\phi}\|^2 - \langle P_i \rangle^2}$. *Then* $\Delta X_i \Delta P_i \geq \frac{\hbar}{2}$ *when* $\|\phi\| = 1$.

Proof. We define $\tilde{X}_i = X_i - \langle X_i \rangle \mathbf{I}$ and $\tilde{P}_i = P_i - \langle P_i \rangle \mathbf{I}$.
Claim: $\tilde{X}_i$ and $\tilde{P}_i$ satisfy Heisenberg's commutation relation. Then apply the above proposition and we are done. □

1.3 Wave Packets in 1D

Now we wish to investigate the wave packets a bit more to find out specific characteristics. We have

$$\phi(t,x) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}} \hat{\phi}_0(k) e^{i(kx - \omega t)} dk,$$

with $\hat{\phi}_0(k) = 0$ for $k \leq 0$.
Goal: Characterize $\langle X \rangle = (X\phi, \phi)$ with $\|\phi\| = 1$ and $\langle P \rangle$ when ϕ satisfies the wave equation. We can factor the wave equation into

$$(\partial_t - c\partial_x)(\partial_t + c\partial_x)\phi = 0.$$

We write the general solution $\phi = \phi_+ + \phi_-$ which correspond to waves traveling forward (backward) denoted with + (-). So now we have

$$\begin{aligned}
\frac{d}{dt}\langle X\rangle &= (X\partial_t\phi, \phi) + (X\phi, \partial_t\phi) \\
&= -2\text{Re}(X\phi, \partial_t\phi) \\
&= -2\text{Re}(X\phi, C\partial_x\phi) \\
&= -2c\text{Re}\int_{\mathbb{R}} x\overline{\phi}\partial_x\phi dx \\
&= -c\int_{\mathbb{R}} x\partial_x|\phi|^2 dx && \text{by integrating by parts, of course} \\
&= c\int_{\mathbb{R}} |\phi|^2 dx = c.
\end{aligned}$$

This means that $\frac{d}{dt}\langle X\rangle = c$. This makes physical sense, since of course a wave should propagate at the speed of light.

Next, we have $\langle P\rangle = \int_{\mathbb{R}} \hbar k|\hat{\phi}(t,k)|^2 dk$. Then $\phi(t,x) = \frac{1}{(2\pi)^{1/2}}\int_{\mathbb{R}} \hat{\phi}_0(k)e^{i(kx-\omega t)}dx$. So $\hat{\phi}(t,k) = \hat{\phi}_0(k)e^{-i\omega t}$. Then $|\hat{\phi}(t,k)|^2 = |\hat{\phi}(k)|^2$ which implies that $\frac{d}{dt}\langle P\rangle = 0$. Physically this is saying that the expected value of the momentum should remain constant, which fits with our classical understanding.

1.4 Dispersive Propagation

Suppose that we have $\omega = \omega(k)$. Then

$$\langle X\langle = (X\phi, \phi) = (X\hat{\phi}, \hat{\phi}),$$

and

$$\hat{X\phi}(k) = i\nabla_k\hat{\phi}.$$

So, $\hat{\phi}(t,k) = \hat{\phi}_0(k)e^{-i\omega(k)t}$ and we have

$$\begin{aligned}
\nabla_k\hat{\phi}(t,k) &= \nabla_k\hat{\phi}_0(k)e^{-i\omega(k)t} - i\nabla_k\omega(k)\hat{\phi}_0(k)e^{-i\omega(k)t} \\
\implies \nabla_k\hat{\phi}\overline{\hat{\phi}} &= \nabla_k\hat{\phi}_0\overline{\hat{\phi}}_0 - i\nabla_k\omega(k)|\hat{\phi}_0(k)|^2 \\
\implies \frac{d}{dt}\langle X\rangle &= \int_{\mathbb{R}^3} \nabla_k\omega(k)|\hat{\phi}_0(k)|^2 dk \\
&= \langle\nabla_k\omega(k)\rangle.
\end{aligned}$$

Note that $\nabla_k\omega(k) = V_g(k)$ is known as the *group velocity*.

So when we have $\omega(k) = ck$ from the wave equation, then we have $\nabla_k\omega(k) = c$ which means there is no dispersion of our wave. As before, we have $\frac{d}{dt}\langle P\rangle = 0$.

With the Schödinger equation, we expect to have the wave disperse. Meaning that the wave packet will widen as time passes. We have $\Delta X_i^2 = \|X_i\phi\|^2 - (\langle X_i\rangle)^2$. Then we claim that $\Delta X_i^2 = At^2 + at + b$.

Exercise. Show that $A = \int_{\mathbb{R}^3} |\nabla_k\omega|^2|\hat{\phi}_0(k)|^2 - \langle V_g\rangle^2$.

From the De Broglie relation we have $E = \frac{\hbar^2|\vec{k}|^2}{2m} = \hbar\omega$ which implies that $\omega(k) = \frac{\hbar|\vec{k}|^2}{2m}$. So we can find that the expression for the wave packet follows from below.

$$\begin{aligned}
\phi(t,x) &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{\phi}_0(k) e^{i\left(k\cdot x - \frac{\hbar|\vec{k}|}{2m} t\right)} dk \\
i\hbar\partial_t \phi &= \frac{\hbar^2}{2m} \int_{\mathbb{R}^3} |k|^2 \hat{\phi}_0(k) e^{i0} dk \\
&= \frac{-\hbar^2}{2m} \Delta\phi.
\end{aligned}$$

This implies the *free Schödinger equation* $i\hbar\partial_t\phi = \frac{-\hbar^2}{2m}\Delta\phi$.

2 References

1. Reed Simon