NONRELATIVISTIC FIELD THEORY - SCHRÖDINGER EQUATION

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References: W. Greiner & J. Reinhardt, *Field Quantization*, Springer-Verlag (1996), Chapter 3, Section 3.2.

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When considering the Lagrangian for the Schrödinger equation we treated the wave function ψ and its complex conjugate ψ^* as the independent variables on which the Lagrangian density $\mathscr{L}$ depends, and we found that the Lagrangian density is given by

$$\mathscr{L}\left(\psi,\nabla\psi,\dot{\psi}\right)=i\hbar\psi^{*}\dot{\psi}-\frac{\hbar^{2}}{2m}\nabla\psi^{*}\cdot\nabla\psi-V\left(\mathbf{x},t\right)\psi^{*}\psi \tag{1}$$

The conjugate momenta are

$$\pi_{1}\left(\mathbf{x},t\right) = \frac{\partial\mathscr{L}}{\partial\dot{\psi}}=i\hbar\psi^{*}\left(\mathbf{x},t\right) \tag{2}$$

$$\pi_{2}\left(\mathbf{x},t\right) = \frac{\partial\mathscr{L}}{\partial\dot{\psi}^{*}}=0 \tag{3}$$

The Poisson brackets containing the fields and their conjugate momenta were derived earlier and are

$$\left\{\psi\left(\mathbf{x},t\right),\pi\left(\mathbf{x}',t\right)\right\}_{PB} = \delta^{3}\left(\mathbf{x}-\mathbf{x}'\right) \tag{4}$$

$$\left\{\phi\left(\mathbf{x},t\right),\phi\left(\mathbf{x}',t\right)\right\}_{PB} = 0 \tag{5}$$

$$\left\{\pi\left(\mathbf{x},t\right),\pi\left(\mathbf{x}',t\right)\right\}_{PB} = 0 \tag{6}$$

To convert to a field theory, we convert the wave function ψ to a field operator $\hat{\psi}$ and its complex conjugate to an adjoint operator $\hat{\psi}^{\dagger}$. The conjugate momentum operator is, from 2

$$\hat{\pi}=i\hbar\hat{\psi}^{\dagger} \tag{7}$$

Using the recipe for converting Poisson brackets to commutators, we have

This relation holds for equal times t.

$$\left\{\psi\left(\mathbf{x},t\right),\pi\left(\mathbf{x}',t\right)\right\}_{PB}\rightarrow\frac{1}{i\hbar}\left[\hat{\psi}\left(\mathbf{x},t\right),\hat{\pi}\left(\mathbf{x}',t\right)\right] \tag{8}$$

From 4 and 7 we have

$$\left[\hat{\psi}(\mathbf{x},t),\hat{\pi}\left(\mathbf{x}',t\right)\right] = \left[\hat{\psi}(\mathbf{x},t),i\hbar\hat{\psi}^{\dagger}\left(\mathbf{x}',t\right)\right] \tag{9}$$

$$= i\hbar\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^{\dagger}\left(\mathbf{x}',t\right)\right] \tag{10}$$

$$= i\hbar\delta^{3}\left(\mathbf{x}-\mathbf{x}'\right) \tag{11}$$

We therefore have the commutator

$$\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^{\dagger}\left(\mathbf{x}',t\right)\right] = \delta^{3}\left(\mathbf{x}-\mathbf{x}'\right) \tag{12}$$

All other commutators are zero.

The time derivative of an operator Q is given by

$$\frac{d\langle\hat{Q}\rangle}{dt} = \frac{1}{i\hbar}\left\langle\left[\hat{Q},H\right]\right\rangle \tag{13}$$

Although this equation was derived by Griffiths directly from nonrelativistic quantum mechanics, we can get the same relation, but for the operators themselves rather than their expectation values, by looking at the Poisson bracket for a classical system, where we found that the time derivative of a classical quantity Q is given by the Poisson bracket of Q with the Hamiltonian:

$$\frac{dQ}{dt} = \{Q,H\} \tag{14}$$

By applying the recipe 8 we get the quantum equivalent

$$\frac{d\hat{Q}}{dt} = \frac{1}{i\hbar}\left[\hat{Q},\hat{H}\right] \tag{15}$$

We therefore have

$$\dot{\hat{\psi}} = \frac{1}{i\hbar}\left[\hat{\psi},\hat{H}\right] \tag{16}$$

$$\dot{\hat{\pi}} = \frac{1}{i\hbar}\left[\hat{\pi},\hat{H}\right] \tag{17}$$

We can find the relation between these two equations as follows. From 7

In the third line, remember that taking the hermitian conjugate also reverses the order of operators in a product. In the last line, we use the fact that $H^{\dagger} = H$

$$\dot{\hat{\pi}} = i\hbar\dot{\hat{\psi}}^\dagger \tag{18}$$
$$= i\hbar\left(\frac{1}{i\hbar}\left[\hat{\psi},\hat{H}\right]\right)^\dagger \tag{19}$$
$$= i\hbar\frac{1}{-i\hbar}\left[\hat{H}^\dagger,\hat{\psi}^\dagger\right] \tag{20}$$
$$= -\left[\hat{H}^\dagger,\hat{\psi}^\dagger\right] \tag{21}$$
$$= \left[\hat{\psi}^\dagger,\hat{H}^\dagger\right] \tag{22}$$
$$= \left[\hat{\psi}^\dagger,\hat{H}\right] \tag{23}$$

[Actually, this relation is fairly obvious from combining 7 and 17 directly, so I don't know why Greiner derives it.]

Finally, we can reclaim the Schrödinger equation from the equation of motion 16, if we recall the form of H from before, but with the parameters now taken to be operators

$$\hat{H} = \int d^3x' \ \hat{\psi}^\dagger\left[-\frac{\hbar^2}{2m}\nabla'^2\hat{\psi} + V\left(\mathbf{x}',t\right)\hat{\psi}\right] \tag{24}$$

We'll use the shorthand notation for the energy operator inside the integral:

$$D_{x'} \equiv -\frac{\hbar^2}{2m}\nabla'^2 + V\left(\mathbf{x}',t\right) \tag{25}$$

We get

$$i\hbar\dot{\hat{\psi}} = \left[\hat{\psi}(\mathbf{x},t),\hat{H}\right] \tag{26}$$
$$= \int d^3x'\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^\dagger\left(\mathbf{x}',t\right)D_{x'}\hat{\psi}\left(\mathbf{x}',t\right)\right] \tag{27}$$

The first term $\hat{\psi}(\mathbf{x},t)$ in the commutator depends on a specific position variable $\mathbf{x}$, while the second term depends on the integration variable $\mathbf{x}'$.

We now use 12 to notice that $\hat{\psi}(\mathbf{x},t)$ commutes with $D_{x'}\hat{\psi}(\mathbf{x}',t)$ but not with $\hat{\psi}^\dagger(\mathbf{x}',t)$, so we can say

$$\left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^\dagger\left(\mathbf{x}',t\right)D_{x'}\hat{\psi}\left(\mathbf{x}',t\right)\right] = \left[\hat{\psi}(\mathbf{x},t),\hat{\psi}^\dagger\left(\mathbf{x}',t\right)\right]D_{x'}\hat{\psi}\left(\mathbf{x}',t\right) \tag{28}$$
$$= \delta^3\left(\mathbf{x}-\mathbf{x}'\right)D_{x'}\hat{\psi}\left(\mathbf{x}',t\right) \tag{29}$$

Plugging this back into the integral and integrating over the delta function gives

$$i\hbar\dot{\hat{\psi}}=\int d^{3}x^{\prime}\delta^{3}\left(\mathbf{x}-\mathbf{x}^{\prime}\right)D_{x^{\prime}}\hat{\psi}\left(\mathbf{x}^{\prime},t\right)=D_{x}\hat{\psi}\left(\mathbf{x},t\right) \tag{30}$$

Written out in full, this is

$$i\hbar\frac{\partial\hat{\psi}}{\partial t}=\left[-\frac{\hbar^{2}}{2m}\nabla^{2}+V\left(\mathbf{x},t\right)\right]\hat{\psi}\left(\mathbf{x},t\right) \tag{31}$$

which is just the Schrödinger equation. Greiner notes that the fact that we got the Schrödinger equation back from the Heisenberg equation of motion 16 isn't fundamental, in the sense that sometimes the field operator $\hat{\psi}$ doesn't satisfy the same differential equation as the original classical field function ψ.

PINGBACKS

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