

Quantum Free Particle Time Evolution

David Chen

September 3, 2012

The time-dependent Schrödinger equation is

$$\hat{\mathcal{H}}(t) |\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle \quad (1)$$

For a time-independent Hamiltonian $\hat{\mathcal{H}}$, the time evolution of the wave-function is

$$|\psi(t)\rangle = e^{-i\frac{\hat{\mathcal{H}}}{\hbar}t} |\psi_0\rangle \quad (2)$$

Projecting it onto $\langle \mathbf{r} |$

$$\langle \mathbf{r} | \psi(t) \rangle = \langle \mathbf{r} | e^{-i\frac{\hat{\mathcal{H}}}{\hbar}t} | \psi_0 \rangle \quad (3)$$

$$= \int d^n r' \underbrace{\langle \mathbf{r} | e^{-i\frac{\hat{\mathcal{H}}}{\hbar}t} | \mathbf{r}' \rangle}_{\equiv \mathcal{K}(\mathbf{r}, \mathbf{r}'; t)} \langle \mathbf{r}' | \psi_0 \rangle \quad (4)$$

where $\mathcal{K}(\mathbf{r}, \mathbf{r}'; t)$ is the *quantum propagator* and n is the dimensionality of space.

In free space, $\hat{\mathcal{H}} = \hat{\mathbf{p}}^2/2m$, therefore ¹

$$\mathcal{K}(\mathbf{r}, \mathbf{r}'; t) = \langle \mathbf{r} | e^{-i\frac{\hat{\mathbf{p}}^2 t}{2m\hbar}} | \mathbf{r}' \rangle \quad (5)$$

$$= \int \langle \mathbf{r} | \mathbf{p}' \rangle d^n p' \langle \mathbf{p}' | e^{-i\frac{\hat{\mathbf{p}}^2 t}{2m\hbar}} | \mathbf{p} \rangle d^n p \langle \mathbf{p} | \mathbf{r}' \rangle \quad (6)$$

$$= \frac{1}{(2\pi\hbar)^n} \int d^n p d^n p' e^{i\frac{\mathbf{r}\cdot\mathbf{p}'}{\hbar}} e^{-i\frac{\mathbf{p}^2 t}{2m\hbar}} \delta(\mathbf{p}' - \mathbf{p}) e^{-i\frac{\mathbf{r}'\cdot\mathbf{p}}{\hbar}} \quad (7)$$

$$= \frac{1}{(2\pi\hbar)^n} \int d^n p e^{-i\frac{\mathbf{p}^2 t}{2m\hbar}} e^{i\frac{\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}{\hbar}} \quad (8)$$

¹ $\langle \mathbf{p}' | \mathbf{r} \rangle = (2\pi\hbar)^{-n/2} e^{-i\frac{\mathbf{r}'\cdot\mathbf{p}}{\hbar}}$; $\langle \mathbf{p}' | e^{-i\frac{\hat{\mathbf{p}}^2 t}{2m\hbar}} | \mathbf{p} \rangle = e^{-i\frac{\mathbf{p}^2 t}{2m\hbar}} \langle \mathbf{p}' | \mathbf{p} \rangle = e^{-i\frac{\mathbf{p}^2 t}{2m\hbar}} \delta(\mathbf{p}' - \mathbf{p})$

Completing the square of the exponent

$$-\frac{it}{2m\hbar} \left(\mathbf{p}^2 - \frac{2m}{t}(\mathbf{r} - \mathbf{r}') \cdot \mathbf{p} \right) = -\frac{it}{2m\hbar} \left(\mathbf{p} - \frac{m}{t}(\mathbf{r} - \mathbf{r}') \right)^2 + \frac{im}{2\hbar t}(\mathbf{r} - \mathbf{r}')^2 \quad (9)$$

Therefore

$$\mathcal{K}(\mathbf{r}, \mathbf{r}'; t) = \frac{1}{(2\pi\hbar)^n} e^{\frac{im}{2\hbar t}(\mathbf{r}-\mathbf{r}')^2} \underbrace{\int d^n p e^{-\frac{it}{2m\hbar} \left(\mathbf{p} - \frac{m}{t}(\mathbf{r}-\mathbf{r}') \right)^2}}_{\left(\frac{2\pi m\hbar}{it} \right)^{n/2}} \quad (10)$$

$$= \left(\frac{m}{2\pi i\hbar t} \right)^{n/2} e^{\frac{im}{2\hbar t}(\mathbf{r}-\mathbf{r}')^2} \quad (11)$$

The following well know property was used in Eq.(10): $\int_{-\infty}^{\infty} e^{-\alpha p^2} = \sqrt{\frac{\pi}{\alpha}} \quad \forall \alpha \in \mathbb{C}, \Re\{\alpha\} > 0$. The exponent of the integrand in Eq.(10) is a pure imaginary number. Strictly speaking, we can not use the property above. However, we can add a positive real number $\epsilon > 0$ in the exponent and then $\epsilon \rightarrow 0$ after integrating.

Finally

$$\boxed{\psi(\mathbf{r}, t) = \left(\frac{m}{2\pi i\hbar t} \right)^{n/2} \int d^n r' e^{\frac{im}{2\hbar t}(\mathbf{r}-\mathbf{r}')^2} \psi_0(\mathbf{r}')} \quad (12)$$

References

- [1] Shankar, R. Principles of Quantum Mechanics, 2nd ed., Chapter 5.
- [2] Pethick, C. J., Bose-Einstein Condensation in Dilute Gases, 2nd ed., Chapter 2