エーレンフェストの定理

量子力学は古典的極限でニュートン力学に一致することが知られています．具体的には，ポテンシャル U の影響下にある，質量 m の粒子が位置 $\boldsymbol{r}$ にあるとき，それぞれの期待値をとれば，ニュートンの運動方程式，

$$m\frac{d^2\boldsymbol{r}}{dt^2} = -\frac{\partial U}{\partial \boldsymbol{r}}$$

が得られるというものです．ここでは，次に示す定理 0.1. と定理 0.2. によってこの事実を示す表題の定理を証明します．なお，$< x >$ は x の期待値を表すものとします．

定理 0.1.

ある粒子の運動量を $\boldsymbol{p}$, 位置を $\boldsymbol{r}$, 質量を m とするとき次の関係式が成り立つ．

$$< \boldsymbol{p} >= m\frac{d}{dt} < \boldsymbol{r} >$$

証明． 成分で書くと定理は次のようになる．

$$< p_x >= m\frac{d}{dt} < x >, < p_y >= m\frac{d}{dt} < y >, < p_z >= m\frac{d}{dt} < z >$$

式の対称性より,x の場合についてだけ証明すれば充分である．まず, 最初にシュレーディンガー方程式より，

$$\begin{aligned}
i\hbar\frac{\partial \Psi}{\partial t} &= -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\Psi + U\Psi \\
\therefore \frac{\partial \Psi}{\partial t} &= \frac{i\hbar}{2m}\boldsymbol{\nabla}^2\Psi - \frac{i}{\hbar}U\Psi \\
\therefore \frac{\partial \Psi^*}{\partial t} &= -\frac{i\hbar}{2m}\boldsymbol{\nabla}^2\Psi^* + \frac{i}{\hbar}U\Psi^*
\end{aligned}$$

だから,

$$
\begin{aligned}
m\frac{d}{dt} < x > &= m\frac{d}{dt}\iiint_{\text{全空間}} \mathit{\Psi}^* x \mathit{\Psi} dxdydz \\
&= m\iiint_{\text{全空間}} \frac{\partial \mathit{\Psi}^*}{\partial t} x\mathit{\Psi} + \mathit{\Psi}^* x \frac{\partial \mathit{\Psi}}{\partial t} dxdydz \\
&= m\iiint_{\text{全空間}} \left(-\frac{i\hbar}{2m}\boldsymbol{\nabla}^2\mathit{\Psi}^* + \frac{i}{\hbar}U\mathit{\Psi}^*\right) x\mathit{\Psi} + \mathit{\Psi}^* x \left(\frac{i\hbar}{2m}\boldsymbol{\nabla}^2\mathit{\Psi} - \frac{i}{\hbar}U\mathit{\Psi}\right) dxdydz \\
&= \iiint_{\text{全空間}} \left(-\frac{i\hbar}{2}\boldsymbol{\nabla}^2\mathit{\Psi}^*\right) x\mathit{\Psi} + \mathit{\Psi}^* x \left(\frac{i\hbar}{2}\boldsymbol{\nabla}^2\mathit{\Psi}\right) dxdydz \\
&= -\frac{i\hbar}{2}\iiint_{\text{全空間}} \left(\frac{\partial^2\mathit{\Psi}^*}{\partial x^2} + \frac{\partial^2\mathit{\Psi}^*}{\partial y^2} + \frac{\partial^2\mathit{\Psi}^*}{\partial z^2}\right) x\mathit{\Psi} - \mathit{\Psi}^* x \left(\frac{\partial^2\mathit{\Psi}}{\partial x^2} + \frac{\partial^2\mathit{\Psi}}{\partial y^2} + \frac{\partial^2\mathit{\Psi}}{\partial z^2}\right) dxdydz \\
&= -\frac{i\hbar}{2}\iiint_{\text{全空間}} \frac{\partial^2\mathit{\Psi}^*}{\partial x^2} x\mathit{\Psi} - \mathit{\Psi}^* x \frac{\partial^2\mathit{\Psi}}{\partial x^2} dxdydz \\
&\quad -\frac{i\hbar}{2}\iiint_{\text{全空間}} \frac{\partial^2\mathit{\Psi}^*}{\partial y^2} x\mathit{\Psi} - \mathit{\Psi}^* x \frac{\partial^2\mathit{\Psi}}{\partial y^2} dxdydz - \frac{i\hbar}{2}\iiint_{\text{全空間}} \frac{\partial^2\mathit{\Psi}^*}{\partial z^2} x\mathit{\Psi} - \mathit{\Psi}^* x \frac{\partial^2\mathit{\Psi}}{\partial z^2} dxdydz \\
&= -i\hbar\iiint_{\text{全空間}} \mathit{\Psi}^* \frac{\partial \mathit{\Psi}}{\partial x} dxdydz \\
&= \iiint_{\text{全空間}} \mathit{\Psi}^* \left(-i\hbar\frac{\partial}{\partial x}\right) \mathit{\Psi} dxdydz \\
&= \iiint_{\text{全空間}} \mathit{\Psi}^* \hat{p_x} \mathit{\Psi} dxdydz \\
&= < p_x >
\end{aligned}
$$

を得る.

なお,

$$\iiint_{全空間} \frac{\partial^2 \Psi^*}{\partial y^2} x\Psi - \Psi^* x \frac{\partial^2 \Psi}{\partial y^2} dxdydz \quad = \quad \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} \frac{\partial^2 \Psi^*}{\partial y^2} x\Psi - \Psi^* x \frac{\partial^2 \Psi}{\partial y^2} dy$$

だから, 部分積分を 2 回用いることにより,

$$\int_{-\infty}^{\infty} \frac{\partial^2 \Psi^*}{\partial y^2} x\Psi dy = \left[\frac{\partial \Psi^*}{\partial y} x\Psi\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial y} x \frac{\partial \Psi}{\partial y} dy = -\int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial y} x \frac{\partial \Psi}{\partial y} dy$$

$$\int_{-\infty}^{\infty} \Psi^* x \frac{\partial^2 \Psi}{\partial y^2} dy = \left[\Psi^* x \frac{\partial \Psi}{\partial y}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial y} x \frac{\partial \Psi}{\partial y} dy = -\int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial y} x \frac{\partial \Psi}{\partial y} dy$$

より, 右辺は 0 になる. 全く同様に, 式の対称性から z の偏微分についての積分も 0 となる. また,

$$\iiint_{全空間} \frac{\partial^2 \Psi^*}{\partial x^2} x\Psi - \Psi^* x \frac{\partial^2 \Psi}{\partial x^2} dxdydz \quad = \quad \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} \frac{\partial^2 \Psi^*}{\partial x^2} x\Psi - \Psi^* x \frac{\partial^2 \Psi}{\partial x^2} dx$$

だから, 部分積分より,

$$\begin{aligned}
\int_{-\infty}^{\infty} \frac{\partial^2 \Psi^*}{\partial x^2} x\Psi dx &= \left[\frac{\partial \Psi^*}{\partial x} x\Psi\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial x} \frac{\partial}{\partial x} (x\Psi)\, dx \\
&= -\int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial x} \Psi dx - \int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial x} x \frac{\partial \Psi}{\partial x} dx \\
&= -\left[\Psi^* \Psi\right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} dx - \int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial x} x \frac{\partial \Psi}{\partial x} dx \\
&= \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} dx - \int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial x} x \frac{\partial \Psi}{\partial x} dx \\
\int_{-\infty}^{\infty} \Psi^* x \frac{\partial^2 \Psi}{\partial x^2} dx &= \left[\Psi^* x \frac{\partial \Psi}{\partial x}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial}{\partial x} (\Psi^* x) \frac{\partial \Psi}{\partial x} dx \\
&= -\int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial x} x \frac{\partial \Psi}{\partial x} dx - \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} dx
\end{aligned}$$

よって,

$$\begin{aligned}
\iiint_{全空間} \frac{\partial^2 \Psi^*}{\partial x^2} x\Psi - \Psi^* x \frac{\partial^2 \Psi}{\partial x^2} dxdydz &= \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} \frac{\partial^2 \Psi^*}{\partial x^2} x\Psi - \Psi^* x \frac{\partial^2 \Psi}{\partial x^2} dx \\
&= \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} 2\Psi^* \frac{\partial \Psi}{\partial x} dx \\
&= 2 \iiint_{全空間} \Psi^* \frac{\partial \Psi}{\partial x} dx
\end{aligned}$$

となる. □

定理 0.2.

ポテンシャル U の影響下にあるある粒子の運動量を $\boldsymbol{p}$, 位置を $\boldsymbol{r}$ とするとき次の関係式が成り立つ.

$$\frac{d}{dt} < \boldsymbol{p} >= - < \frac{\partial U}{\partial \boldsymbol{r}} >$$

証明. 成分で書くと定理は次のようになる.

$$\frac{d}{dt} < p_x >= - < \frac{\partial U}{\partial x} >, \frac{d}{dt} < p_y >= - < \frac{\partial U}{\partial y} >, \frac{d}{dt} < p_z >= - < \frac{\partial U}{\partial z} >$$

式の対称性より,x の場合についてだけ証明すれば充分である.

$$\begin{aligned}
\frac{d}{dt} < p_x > &= \frac{d}{dt} \iiint_{\text{全空間}} \Psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi dxdydz \\
&= \iiint_{\text{全空間}} -i\hbar \frac{\partial \Psi^*}{\partial t} \frac{\partial \Psi}{\partial x} + \Psi^* \left(-\frac{\partial}{\partial x} \right) \left(i\hbar \frac{\partial \Psi}{\partial t} \right) dxdydz \\
&= \iiint_{\text{全空間}} \left(-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 \Psi^* + U\Psi^* \right) \frac{\partial \Psi}{\partial x} + \Psi^* \left(-\frac{\partial}{\partial x} \right) \left(-\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 \Psi + U\Psi \right) dxdydz \\
&= \frac{\hbar^2}{2m} \iiint_{\text{全空間}} \Psi^* \frac{\partial}{\partial x} (\boldsymbol{\nabla}^2 \Psi) - \boldsymbol{\nabla}^2 \Psi^* \frac{\partial \Psi}{\partial x} dxdydz - \iiint_{\text{全空間}} \Psi^* \frac{\partial U}{\partial x} \Psi dxdydz \\
&= - \left\langle \frac{\partial U}{\partial x} \right\rangle
\end{aligned}$$

なお,

$$\begin{aligned}
& \iiint_{\text{全空間}} \Psi^* \frac{\partial}{\partial x} (\boldsymbol{\nabla}^2 \Psi) - \boldsymbol{\nabla}^2 \Psi^* \frac{\partial \Psi}{\partial x} dxdydz \\
= & \iiint_{\text{全空間}} \Psi^* \frac{\partial}{\partial x} \left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) - \left(\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{\partial^2 \Psi^*}{\partial y^2} + \frac{\partial^2 \Psi^*}{\partial z^2} \right) \frac{\partial \Psi}{\partial x} dxdydz \\
= & \iiint_{\text{全空間}} \Psi^* \frac{\partial}{\partial x} \frac{\partial^2 \Psi}{\partial x^2} - \frac{\partial^2 \Psi^*}{\partial x^2} \frac{\partial \Psi}{\partial x} dxdydz \\
& + \iiint_{\text{全空間}} \Psi^* \frac{\partial}{\partial x} \frac{\partial^2 \Psi}{\partial y^2} - \frac{\partial^2 \Psi^*}{\partial y^2} \frac{\partial \Psi}{\partial x} dxdydz \\
& + \iiint_{\text{全空間}} \Psi^* \frac{\partial}{\partial x} \frac{\partial^2 \Psi}{\partial z^2} - \frac{\partial^2 \Psi^*}{\partial z^2} \frac{\partial \Psi}{\partial x} dxdydz \\
= & \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} \Psi^* \frac{\partial}{\partial x} \frac{\partial^2 \Psi}{\partial x^2} - \frac{\partial^2 \Psi^*}{\partial x^2} \frac{\partial \Psi}{\partial x} dx \\
& \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} \Psi^* \frac{\partial}{\partial x} \frac{\partial^2 \Psi}{\partial y^2} - \frac{\partial^2 \Psi^*}{\partial y^2} \frac{\partial \Psi}{\partial x} dy \\
& \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} \Psi^* \frac{\partial}{\partial x} \frac{\partial^2 \Psi}{\partial z^2} - \frac{\partial^2 \Psi^*}{\partial z^2} \frac{\partial \Psi}{\partial x} dz
\end{aligned}$$

となる. ここで,

$$
\begin{aligned}
\int_{-\infty}^{\infty} \Psi^* \frac{\partial}{\partial x} \frac{\partial^2 \Psi}{\partial x^2} dx &= \left[\Psi^* \frac{\partial^2 \Psi}{\partial x^2} \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial x} \frac{\partial^2 \Psi}{\partial x^2} dx \\
&= - \left[\frac{\partial \Psi^*}{\partial x} \frac{\partial \Psi}{\partial x} \right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{\partial^2 \Psi^*}{\partial x^2} \frac{\partial \Psi}{\partial x} dx \\
&= \int_{-\infty}^{\infty} \frac{\partial^2 \Psi^*}{\partial x^2} \frac{\partial \Psi}{\partial x} dx
\end{aligned}
$$

また同様に,

$$
\begin{aligned}
\int_{-\infty}^{\infty} \Psi^* \frac{\partial}{\partial x} \frac{\partial^2 \Psi}{\partial y^2} dy &= \left[\Psi^* \frac{\partial^2 \Psi}{\partial x \partial y} \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial y} \frac{\partial^2 \Psi}{\partial x \partial y} dy \\
&= - \left[\frac{\partial \Psi^*}{\partial y} \frac{\partial \Psi}{\partial x} \right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{\partial^2 \Psi^*}{\partial y^2} \frac{\partial \Psi}{\partial x} dy \\
&= \int_{-\infty}^{\infty} \frac{\partial^2 \Psi^*}{\partial y^2} \frac{\partial \Psi}{\partial x} dy
\end{aligned}
$$

式の対象性から全く同様のことが z についても成り立つ. 以上より,

$$
\iiint_{\text{全空間}} \Psi^* \frac{\partial}{\partial x} (\boldsymbol{\nabla}^2 \Psi) - \boldsymbol{\nabla}^2 \Psi^* \frac{\partial \Psi}{\partial x} dx dy dz = 0
$$

が示せた. □

以上,2 つの定理より次の定理が成り立つことが分かる.

定理 0.3. エーレンフェストの定理

ポテンシャル U の影響下にあるある粒子の位置を $\boldsymbol{r}$, 質量を m とするとき次の関係式が成り立つ.

$$
m \frac{d^2}{dt^2} < \boldsymbol{r} >= - \left\langle \frac{\partial U}{\partial \boldsymbol{r}} \right\rangle
$$