

量子化学原理与应用笔记

L^AT_EX 模板

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2021 年 9 月 30 日

1 公式

有编号公式

$$\hat{A}u = v \quad (1)$$

无编号公式

$$cu, fu, \frac{\partial}{\partial x}u, \sqrt{u}$$

多行公式，分别编号

$$\langle A \rangle = \int \psi^* \hat{A} \psi dx \quad (2)$$

$$\langle A \rangle^* = \left(\int \psi^* \hat{A} \psi dx \right)^* = \int (\hat{A} \psi)^* \psi dx \quad (3)$$

多行公式，只编号一次

$$\begin{aligned} \frac{\partial}{\partial t} |\Psi(x, t)|^2 &= \frac{\partial \Psi^*}{\partial t} \Psi + \Psi^* \frac{\partial \Psi}{\partial t} = \Psi \left(-\frac{i\hbar}{2m} \frac{\partial^2}{\partial x^2} \Psi + \frac{i}{\hbar} V(x) \Psi \right) + \Psi^* \left(\frac{i\hbar}{2m} \frac{\partial^2}{\partial x^2} \Psi - \frac{i}{\hbar} V(x) \Psi \right) \\ &= \frac{i\hbar}{2m} \left[\Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \Psi \frac{\partial^2 \Psi^*}{\partial x^2} \right] \\ &= \frac{i\hbar}{2m} \frac{\partial}{\partial x} \left[\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right] \end{aligned} \quad (4)$$

有编号列表

1. 和与差
2. 乘法
3. 等价算符
4. 基本算符
5. 逆
6. 对易子

无编号列表

- 三维: $s < \frac{3}{2}$
- 二维: $s < 1$
- 一维: $s < \frac{1}{2}$

1.1 数学和物理符号

基本符号

$\$ \backslash \text{hbar}, \backslash \text{oint}, \backslash \text{prod}, \backslash \text{forall}, \backslash \text{nabla}, \backslash \text{cdots}, \backslash \text{therefore} \$ \backslash$

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2 $ \hat A , \mathbb{R}, \Re, \ell$\\
3 $ \neq, \gg, \ll, \approx, \propto, \rightarrow, \Rightarrow, \leftrightarrow$\\
4 $ \sin, \arcsin, \sinh, \ln, \exp $

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$\hbar, \oint, \prod, \forall, \nabla, \cdots, \therefore$
 $\hat{A}, \mathbb{R}, \Re, \ell$
 $\neq, \gg, \ll, \approx, \propto, \rightarrow, \Rightarrow, \leftrightarrow$
 $\sin, \arcsin, \sinh, \ln, \exp$

physics 包中的符号

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1 \begin{equation}
2 \dv{x}, \dv{\psi}{x}, \dv[2]{\psi}{x}, \pdv{x}, \pdv[2]{x} , \int \dd x
3 \end{equation}
4 \begin{equation}
5 \bra{\varphi}, \ket{\phi}, \ev{\hat p}
6 \end{equation}
7 \begin{equation}
8 \qty( \dfrac{x}{y} ), \qty[ \dfrac{x}{y} ], \qty{ \dfrac{x}{y} }, \qty| \dfrac{x}{y} |
9 \end{equation}
10 \begin{equation}
11 \mqty( a \& b \& c \& d ), \mqty| a \& b \& c \& d |
12 \end{equation}

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$$\frac{d}{dx}, \frac{d\psi}{dx}, \frac{d^2\psi}{dx^2}, \frac{\partial}{\partial x}, \frac{\partial^2}{\partial x^2}, \int dx \quad (5)$$

$$\langle \varphi |, | \phi \rangle, \langle \hat{p} \rangle \quad (6)$$

$$\left(\frac{x}{y}\right), \left[\frac{x}{y}\right], \left\{\frac{x}{y}\right\}, \left|\frac{x}{y}\right| \quad (7)$$

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \begin{vmatrix} a & b \\ c & d \end{vmatrix} \quad (8)$$

Braket 包中的符号

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1 \begin{equation}\label{braket}
2 \Braket{\psi | \pdv{x} | \psi}
3 \end{equation}

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$$\left\langle \phi \left| \frac{\partial}{\partial x} \right| \phi \right\rangle \quad (9)$$

2 插入 block

Note

为什么我们需要特别引入 Hermitian 算符？

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Warning

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3 杂项

脚注

Note

但是在量子力学中并不排除会使用某些不能归一化的波函数。^a

^a这是一个脚注

引用公式, (9)。需要多编译一次。

4 一些自定义命令