

量子化学原理与应用笔记

L^AT_EX 模板

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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 $\hat{A}, \alpha, \rightarrow$

physics 包中的符号

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

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

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

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

Braket 包中的符号

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

1.2 插入 block

Note

为什么我们需要特别引入 Hermitian 算符？

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Warning

但需要留意的是，Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

1.3 一些自定义命令

近乎

2 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，(8)。需要多编译一次。