量子化学原理与应用笔记
LaTeX 模板

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1 公式

有编号公式

$$\hat{A}u = v \tag{1}$$

无编号公式

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

多行公式，分别编号

$$\langle A\rangle = \int \psi^* \hat{A}\psi \mathrm{d}x \tag{2}$$

$$\langle A\rangle^* = \left(\int \psi^* \hat{A}\psi \mathrm{d}x\right)^* = \int (\hat{A}\psi)^*\psi \mathrm{d}x \tag{3}$$

多行公式，只编号一次

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

单行多行混合公式

$$V(x) = \begin{cases} 0, & x \in (-\infty, 0) \quad \text{Block I} \\ V_0, & x \in [0, l] \quad \text{Block II} \\ 0, & x \in (l, +\infty) \quad \text{Block III} \end{cases} \tag{5}$$

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

```
$ \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 $
```

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

physics 包中的符号

```
\begin{equation}
\dv{x}, \dv{\psi}{x}, \dv[2]{\psi}{x}, \pdv{x}, \pdv[2]{x} , \int \dd x
\end{equation}
\begin{equation}
\bra{\varphi}, \ket{\phi}, \ev{\hat p}
\end{equation}
\begin{equation}
\qty(  \dfrac{x}{y} ), \qty[ \dfrac{x}{y} ], \qty{\dfrac{x}{y} }, \qty| \dfrac{x}{y} |
\end{equation}
\begin{equation}
\mqty( a & b \\ c & d ), \mqty| a & b \\ c & d |
\end{equation}
```

$$\frac{\mathrm{d}}{\mathrm{d}x}, \frac{\mathrm{d}\psi}{\mathrm{d}x}, \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}, \frac{\partial}{\partial x}, \frac{\partial^2}{\partial x^2}, \int \mathrm{d}x \tag{6}$$

$$\langle\varphi|, |\phi\rangle, \langle\hat{p}\rangle \tag{7}$$

$$\left(\frac{x}{y}\right), \left[\frac{x}{y}\right], \left\{\frac{x}{y}\right\}, \left|\frac{x}{y}\right| \tag{8}$$

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \begin{vmatrix} a & b \\ c & d \end{vmatrix} \tag{9}$$

Braket 包中的符号

```
\begin{equation}\label{braket}
\Braket{\phi | \pdv{x} | \phi}
\end{equation}
```

$$\left\langle \phi \middle| \frac{\partial}{\partial x} \middle| \phi \right\rangle \tag{10}$$

2 插入 block

Note

为什么我们需要特别引入 Hermitian 算符？

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

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.

3 插入图表

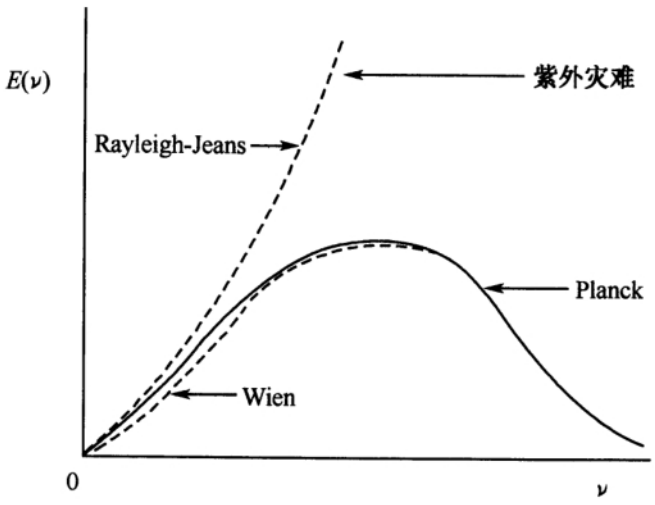
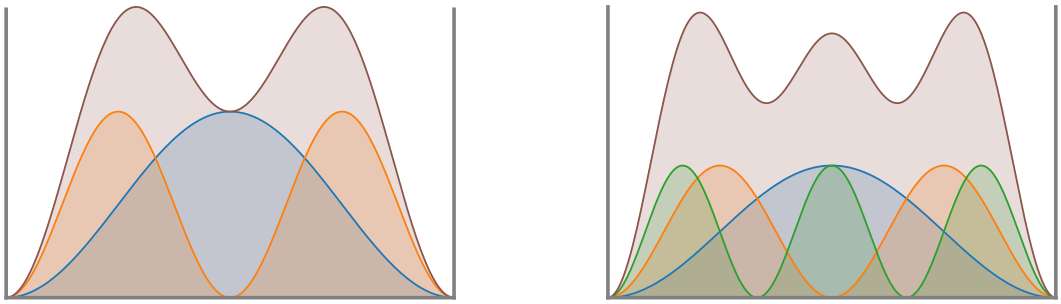


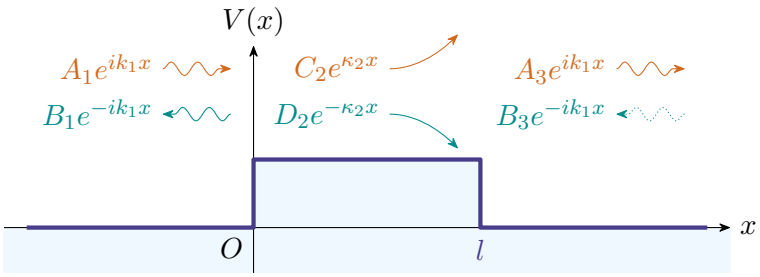
图 1: 这是一张图



(a) 1,3-丁二烯　　**(b)** 1,3,5-己三烯

图 2: 这是两张图

3.1 TikZ 图



4 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，(10)。需要多编译一次。

4.1 一些自定义命令