$$(\sigma\cdot P)V(\sigma\cdot P)$$

$$
\begin{aligned}
= {} & I_2 P_x V P_x + I_2 P_y V P_y + I_2 P_z V P_z \\
& + i\sigma_z (P_x V P_y - P_y V P_x) \\
& + i\sigma_y (P_x V P_z - P_z V P_x) \\
& + i\sigma_x (P_y V P_z - P_z V P_y)
\end{aligned}
$$

$$\sqrt{\frac{\epsilon_i\epsilon_j}{\epsilon_k}}(\sigma\cdot P)V\sqrt{\frac{\epsilon_i\epsilon_j}{\epsilon_k}}(\sigma\cdot P)$$ V的两边对称,算符厄米

$$
\begin{aligned}
= {} & I_2\sqrt{\frac{\epsilon_y\epsilon_z}{\epsilon_x}}P_x V\sqrt{\frac{\epsilon_y\epsilon_z}{\epsilon_x}}P_x + I_2\sqrt{\frac{\epsilon_x\epsilon_z}{\epsilon_y}}P_y V\sqrt{\frac{\epsilon_x\epsilon_z}{\epsilon_y}}P_y + I_2\sqrt{\frac{\epsilon_x\epsilon_y}{\epsilon_z}}P_z V\sqrt{\frac{\epsilon_x\epsilon_y}{\epsilon_z}}P_z \\
& + i\sigma_z\left(\sqrt{\frac{\epsilon_y\epsilon_z}{\epsilon_x}}P_x V\sqrt{\frac{\epsilon_x\epsilon_z}{\epsilon_y}}P_y - \sqrt{\frac{\epsilon_x\epsilon_z}{\epsilon_y}}P_y V\sqrt{\frac{\epsilon_y\epsilon_z}{\epsilon_x}}P_x\right) \\
& + i\sigma_y\left(\sqrt{\frac{\epsilon_y\epsilon_z}{\epsilon_x}}P_x V\sqrt{\frac{\epsilon_x\epsilon_y}{\epsilon_z}}P_z - \sqrt{\frac{\epsilon_x\epsilon_y}{\epsilon_z}}P_z V\sqrt{\frac{\epsilon_y\epsilon_z}{\epsilon_x}}P_x\right) \\
& + i\sigma_x\left(\sqrt{\frac{\epsilon_x\epsilon_z}{\epsilon_y}}P_y V\sqrt{\frac{\epsilon_x\epsilon_y}{\epsilon_z}}P_z - \sqrt{\frac{\epsilon_x\epsilon_y}{\epsilon_z}}P_z V\sqrt{\frac{\epsilon_x\epsilon_z}{\epsilon_y}}P_y\right)
\end{aligned}
$$

$$\epsilon_x = \frac{1}{\sqrt{1-\frac{c^2}{\epsilon^2}P_x^2}} = 1+\frac{P_x^2}{2c^2} \qquad (到\ c^{-2}\ 阶)$$

$$\therefore \sqrt{\frac{\epsilon_y\epsilon_z}{\epsilon_x}} = 1+\frac{P_y^2}{4c^2}+\frac{P_z^2}{4c^2}-\frac{P_x^2}{4c^2} = 1+\frac{1}{4c^2}(P^2-2P_x^2) \qquad (到\ c^{-2}\ 阶)$$

以 $\sqrt{\frac{\epsilon_y\epsilon_z}{\epsilon_x}}P_x V\sqrt{\frac{\epsilon_y\epsilon_z}{\epsilon_x}}P_x$ 为例,化为:

$$\left[1+\frac{1}{4c^2}(P^2-2P_x^2)\right]P_x V\left[1+\frac{1}{4c^2}(P^2-2P_x^2)\right]P_x$$

$$\left[1+\frac{1}{4c^2}(p^2-2p_x^2)\right]p_x V\left[1+\frac{1}{4c^2}(p^2-2p_x^2)\right]p_x$$

$$=p_xVp_x+\frac{1}{4c^2}(p^2-2p_x^2)p_xVp_x+\frac{1}{4c^2}p_xVp_x(p^2-2p_x^2) \quad (\text{到 } c^{-2} \text{阶})$$

$$=p_xVp_x+\frac{1}{4c^2}p^2p_xVp_x+\frac{1}{4c^2}p_xVp_xp^2$$

$$-\frac{1}{2c^2}p_x^2p_xVp_x-\frac{1}{2c^2}p_xVp_x^2p_x$$

p^2用$\langle p^2\rangle$本征空间描述.

所以要算的有:

p_xVp_x、p_yVp_y、p_zVp_z、$p_x^3Vp_x$、$p_xVp_x^3$、$p_y^3Vp_y$、$p_yVp_y^3$、$p_z^3Vp_z$、$p_zVp_z^3$

p_xVp_y、p_yVp_x、$p_x^3Vp_y$、$p_xVp_y^3$、$p_y^3Vp_x$、$p_yVp_x^3$

p_xVp_z、p_zVp_x、$p_x^3Vp_z$、$p_xVp_z^3$、$p_z^3Vp_x$、$p_zVp_x^3$

p_zVp_y、p_yVp_z、$p_z^3Vp_y$、$p_zVp_y^3$、$p_y^3Vp_z$、$p_yVp_z^3$

共27个pVp矩阵元! 这些矩阵元之间不可约分.

$$(\langle\chi_i|p_xVp_z|\chi_j\rangle)^\dagger \overset{实}{=} p_xVp_z|_{ij}$$

$$=\langle\chi_j|p_zVp_x|\chi_i\rangle$$

$$=p_zVp_x|_{ji}$$

$$(\langle\chi_i|p_x^3Vp_z|\chi_j\rangle)^\dagger \overset{实}{=} p_x^3Vp_z|_{ij}$$

$$=\langle\chi_j|p_zVp_x^3|\chi_i\rangle$$

$$=p_zVp_x^3|_{ji}$$

pVp和p^3Vp、pVp^3
都是非对称实矩阵
但都只需算半对角.

$\langle \chi_i | P_x V P_z | \chi_j \rangle$

$= \langle \chi_i | (-i\partial_x)^\dagger V -i\partial_z | \chi_j \rangle$

$= \langle \chi_i | -i\partial_x V -i\partial_z | \chi_j \rangle$

$= -\langle \chi_i | \partial_x V \partial_z | \chi_j \rangle$

P^2、PVP 要取负

$\langle \chi_i | P_x^3 V P_z | \chi_j \rangle$

$= \langle \chi_i | (-i\partial_x)^{3\dagger} V -i\partial_z | \chi_j \rangle$

$= \langle \chi_i | -i\cdot(-\partial_x^3) V -i\partial_z | \chi_j \rangle$

$= \langle \chi_i | \partial_x^3 V \partial_z | \chi_j \rangle$

P^3VP、PVP^3 不取负.

注意:

$$\langle \chi_i | \partial_x^\dagger \partial_x | \chi_j \rangle = \int dx \langle \chi_i | \partial_x^\dagger | x \rangle \langle x | \partial_x | \chi_j \rangle$$

$$= \int dx \left(\frac{\partial}{\partial x}\chi_i(x)\right)\left(\frac{\partial}{\partial x}\chi_j(x)\right)$$

$$\langle \chi_i | \partial_x \partial_x | \chi_j \rangle = \int dx \langle \chi_i | x \rangle \langle x | \frac{\partial^2}{\partial x^2} | \chi_j \rangle$$

$$= \int dx\, \chi_i(x) \frac{\partial^2}{\partial x^2}\chi_j(x)$$

$$= \int d\left(\frac{\partial}{\partial x}\chi_j(x)\right) \chi_i(x)$$

$$= \chi_i(x)\frac{\partial}{\partial x}\chi_j(x)\Big|_{-\infty}^{+\infty} - \int dx \frac{\partial}{\partial x}\chi_j(x)\frac{\partial}{\partial x}\chi_i(x)$$

$$\overset{\text{边条}}{=} -\int dx \frac{\partial}{\partial x}\chi_j(x)\frac{\partial}{\partial x}\chi_i(x)$$

$$= -\langle \chi_i | \partial_x^\dagger \partial_x | \chi_j \rangle$$

所以用两边作用方式计算的其实正是 $-\nabla^2$ 阵, 不用再取负.

故: $\langle \chi_i | P_x V P_z | \chi_j \rangle = -\langle \chi_i | \partial_x V \partial_z | \chi_j \rangle = \langle \chi_i | \partial_x^\dagger V \partial_z | \chi_j \rangle$ P^2、pVp 不取负

$\langle \chi_i | P_x^3 V P_z | \chi_j \rangle = \langle \chi_i | \partial_x^3 V \partial_z | \chi_j \rangle = -\langle \chi_i | \partial_x^{3\dagger} V \partial_z | \chi_j \rangle$ p^3Vp、pVp^3 要取负