

h\_psi evaluation

$\nabla^2$

$u(\mathbf{G})$

$$-\frac{1}{2} |\mathbf{G} + \mathbf{k}|^2 u(\mathbf{G}), \forall \mathbf{G}$$

IFFT

$u(\mathbf{r})$

$v_{eff}$

$$v_{eff}(\mathbf{r}) \cdot u(\mathbf{r}), \forall \mathbf{r}$$

FFT

$$(v_{eff} u)(\mathbf{G})$$

$$(\mathbf{H}^{KS} \cdot u)(\mathbf{G})$$

