

GRAPE Scheme

$$J = 1 - \left| \frac{1}{4} \sum_n \underbrace{\langle \psi_n(\tau) | \psi_n^{(tgt)} \rangle}_{\equiv \tau_n} \right|^2$$

$$= 1 - \frac{1}{16} \sum_{nn'} \tau_{n'}^* \tau_n$$

$$\frac{\partial J}{\partial E_{nl}} = -\frac{1}{16} \sum_{nl} \left(\frac{\partial \tau_{nl}^*}{\partial E_{nl}} \tau_{nl} + \tau_{nl}^* \frac{\partial \tau_{nl}}{\partial E_{nl}} \right)$$

$$= -\frac{2}{16} \operatorname{Re} \left[\sum_{nn'} \tau_{nl}^* \frac{\partial \tau_{nl}}{\partial E_{nl}} \right]$$