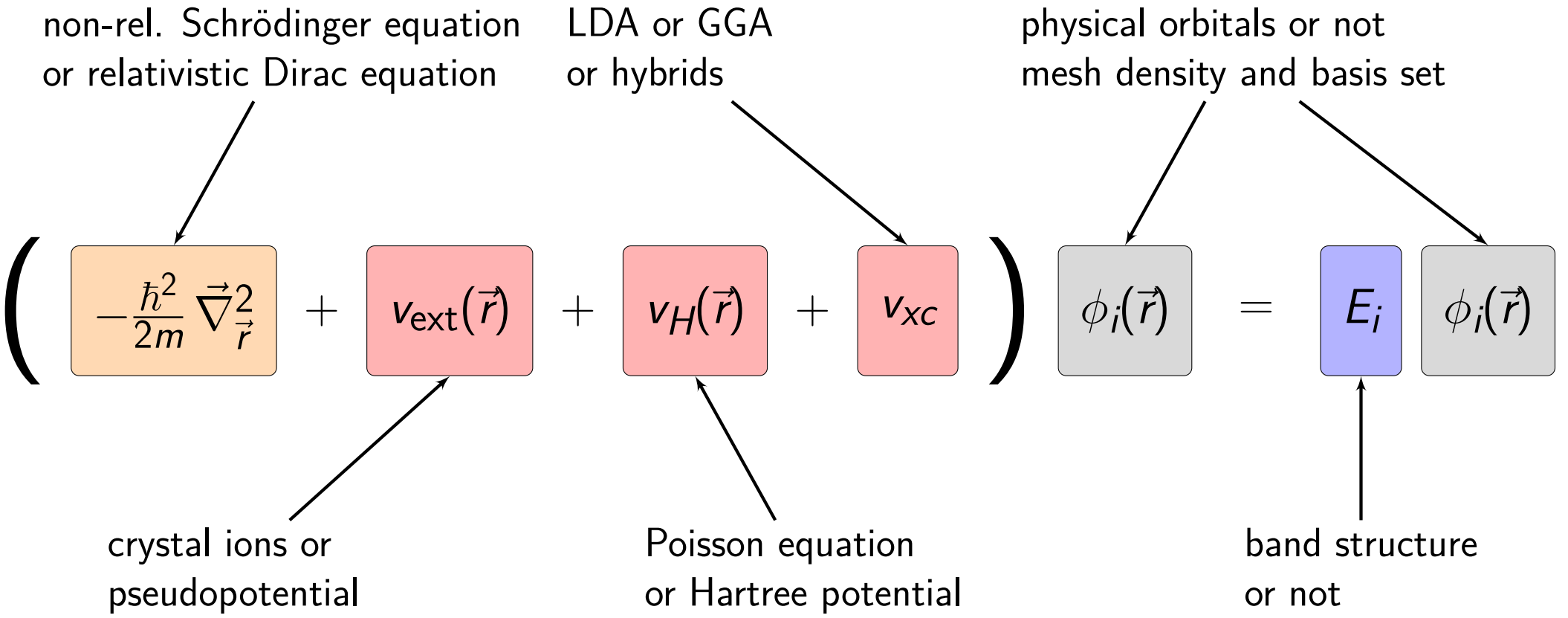
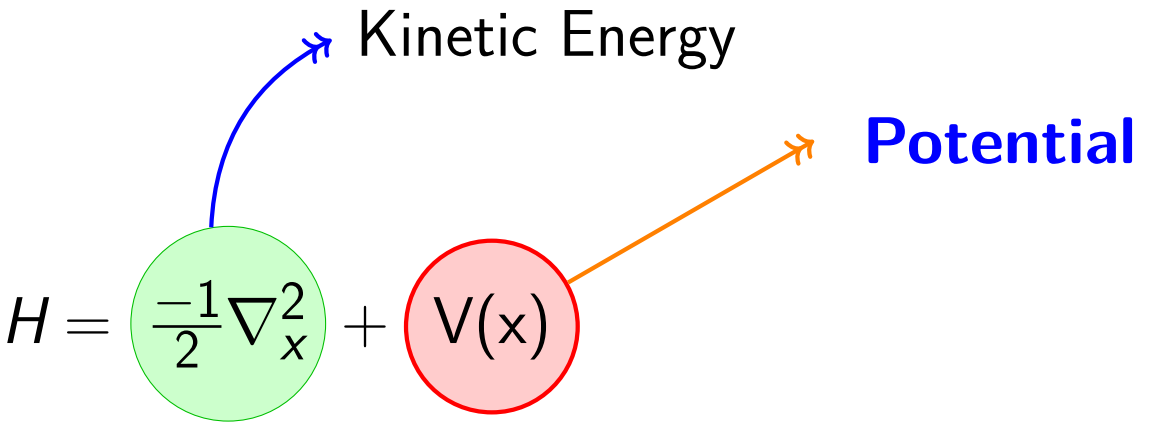
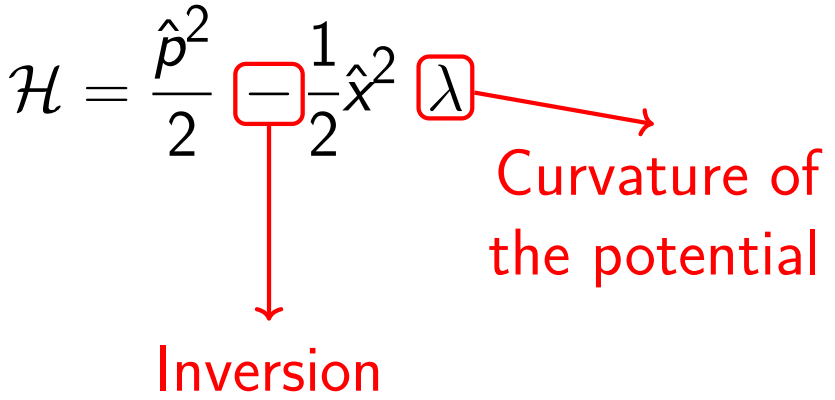

non-rel. Schrödinger equation
or relativistic Dirac equation
LDA or GGA
or hybrids
physical orbitals or not
mesh density and basis set
$\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2_{\vec{r}} + v_{\text{ext}}(\vec{r}) + v_H(\vec{r}) + v_{xc} \right) \phi_i(\vec{r}) = E_i \phi_i(\vec{r})$
crystal ions or
pseudopotential
Poisson equation
or Hartree potential
band structure
or not


Kinetic Energy
Potential
$H = \frac{-1}{2}\nabla_x^2 + V(x)$

$$\hat{A}(t) = \underbrace{e^{\frac{iHt}{\hbar}}}_{\text{Backward}} \underbrace{\hat{A}}_{\text{Perturbation}} \underbrace{e^{\frac{-iHt}{\hbar}}}_{\text{Forward}}$$

$$\hat{\mathcal{H}}\psi(x) = \underbrace{\left(-\frac{1}{2}\nabla_x^2 - \frac{1}{2}\hat{x}^2\lambda\right)\psi(x)}_{\text{Scattering off a parabolic potential barrier}} = E\psi(x)$$


$\mathcal{H} = \frac{\hat{p}^2}{2} - \frac{1}{2}\hat{x}^2 \lambda$
Curvature of
the potential
Inversion