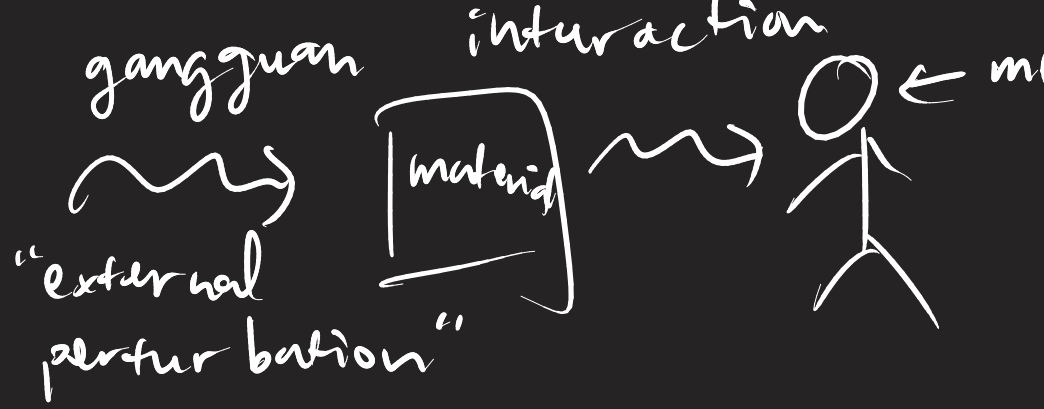
- Teori kuantum
  - elektron : potensial sederhana
  - atom : hidrogen, Born-Oppenheimer
  - molekul : LCAO
  - kristal : TB model, DFT, dll..

- Sifat2 material : interaksi / gangguan



observables :

$$\langle \hat{O} \rangle = \langle \psi | \hat{H} | \psi \rangle$$

$$O_{i \to f} = \langle \psi_f | H_{int} | \psi_i \rangle$$

intensitas : $I \propto |O|^2$

$S : [V/K]$

$\sigma : [1/m\Omega]$

$\kappa : (W/mK)$

$PF = S^2 \sigma$

$(PF) = \frac{V^2}{K^2} \cdot \frac{1}{\Omega}$

$= \frac{W}{mK^2}$

$(ZT) = \frac{(S^2 \sigma)}{[\kappa]} \cdot (T)$

$= \frac{W/mK^2}{W/mK} \cdot K$

$= 1$ (dimensionless)

efficiency:

$\eta = \frac{P_{output}}{P_{input}} \times 100\%$

- Sifat termoelektrik ingredients ↓ perhitungan

$\varepsilon(k)$: energy dispersion

DOS $[g(\varepsilon)]$ density of states

$\varepsilon = \hbar\omega$

v : group velocity.

$$v = \frac{d\omega}{dk} = \frac{1}{\hbar} \frac{d\varepsilon}{dk}$$