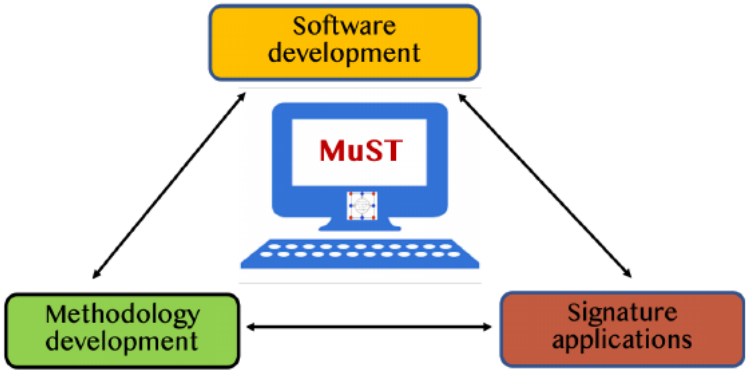
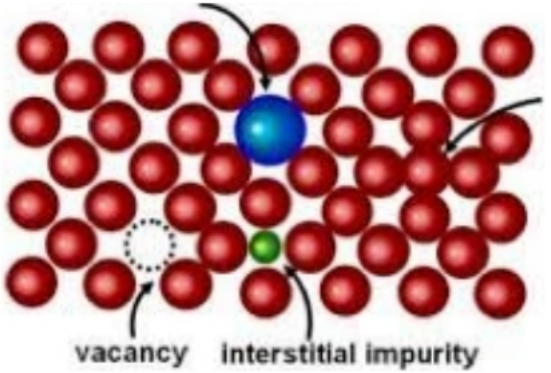
THEORY



MATERIALS



COMPUTATION

MuST STUDENT WORKSHOP 2023

June 27, 2023

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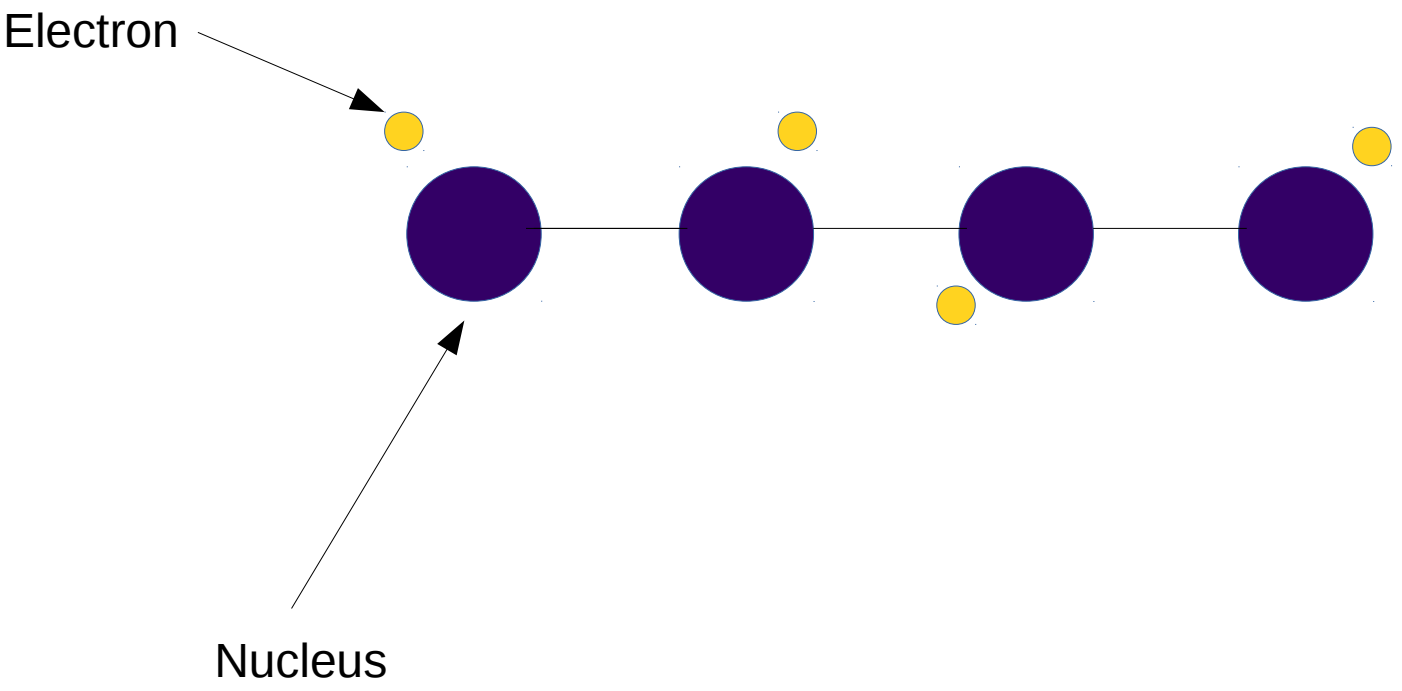
Hamiltonian of a system with interacting nuclei and electrons

$$H = T_e + V_{e-N} + V_{e-e} + T_N + V_{N-N}$$



Hamiltonian Matrix:

- H = K.E. + P.E
- K.E. = Off diagonal values of the matrix which we call hopping t. (Usually a negative number).
- P.E = The diagonal elements of the matrix (randomly uniformed distributed umbers between to set of numbers times the W).

Time dependent Schrödinger's equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(r,t) + V(r,t)\Psi(r,t) = i\hbar\frac{\partial\Psi(r,t)}{\partial t}$$

Wavefunction as a function of electrons, nuclei, and time

$$\Psi(r,t) = \Psi(r_1, r_2, \cdots, R_1, R_2, \cdots, t)$$

Time independent potential

$$V(r,t) = V(r,t=0)$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r) + V(r)\psi(r) = E\psi(r)$$

Fix nuclei, only treat electrons quantum mechanically

$$\psi(r) = \psi(r_1, r_2, \cdots, t)$$

Hamiltonian for electrons with fixed nuclei

$$H = T + V + U$$

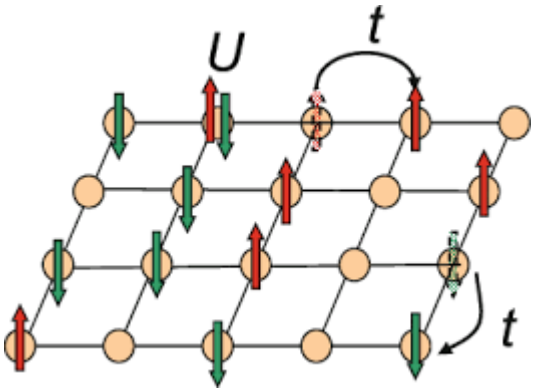
$$H = -\frac{1}{2}\sum_j \nabla_j^2 + \sum_j v(r_j) + \frac{1}{2}\sum_{i \neq j} \frac{1}{|r_i - r_j|}$$

Hubbard Model

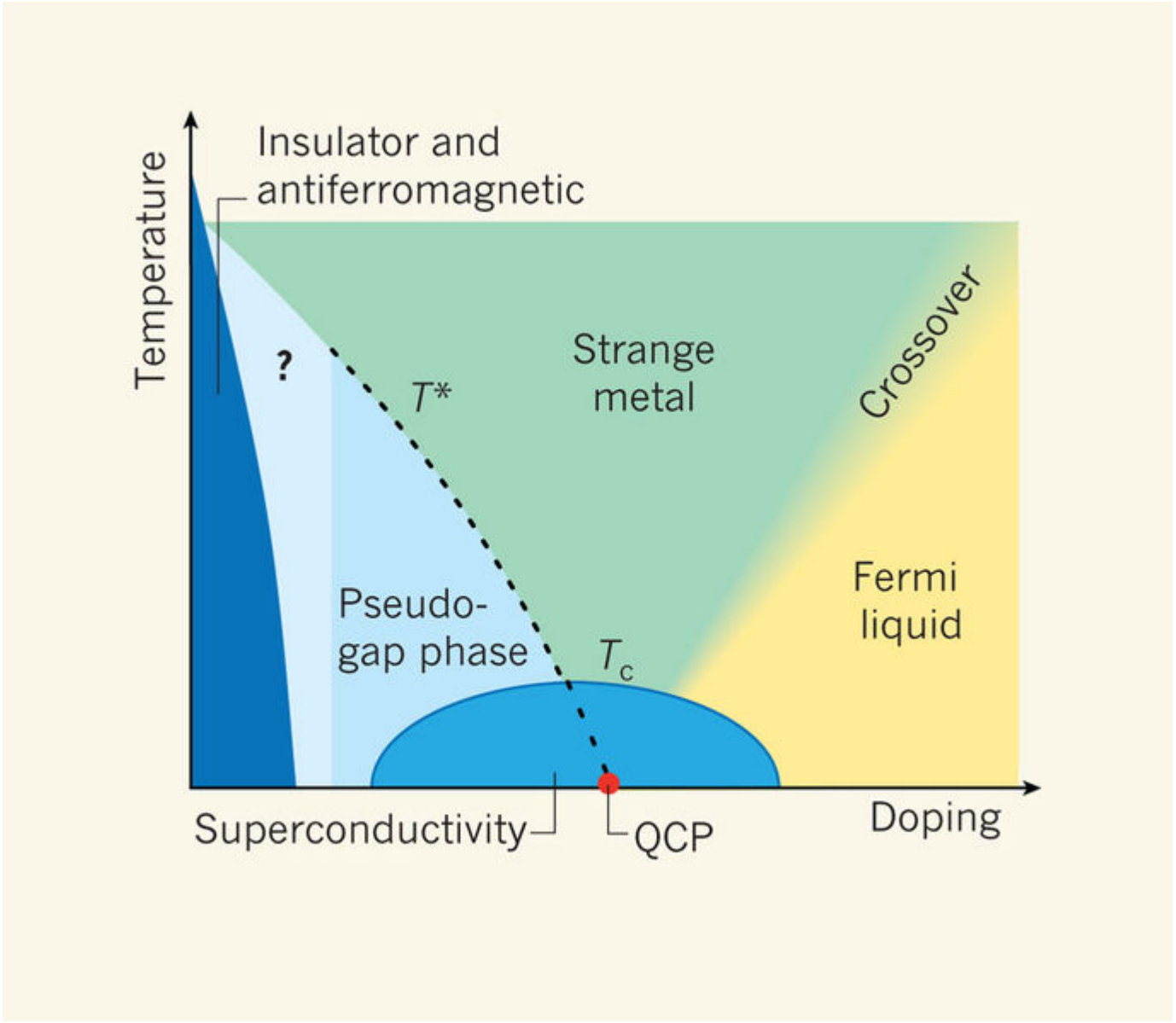
$$H = -\sum_{<ij>} t\left(c_{i\sigma}^{+} c_{j\sigma} + H.C.\right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

- Hamiltonian which accounts for electron-electron interaction

- Can capture interesting features similar to those found in Cuprates



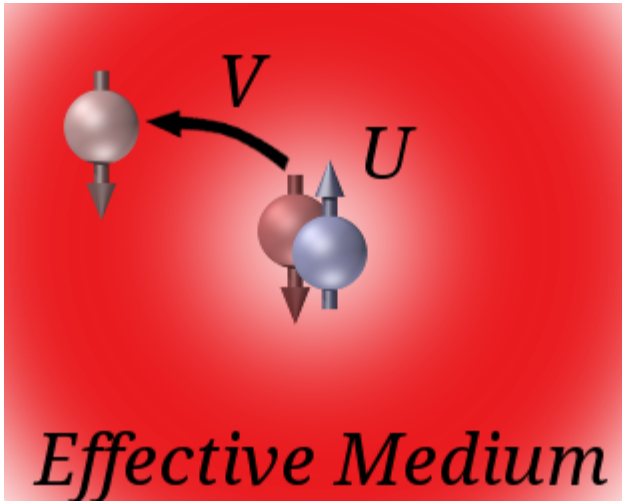
Picture from Wikipedia



C. Varma
https://www.nature.com/articles/468184a

Hubbard Model Infinite Dimensions

- Dynamical Mean Field Approximation



Picture from Devereaux group

- Equivalent to single site Anderson Model

$$H_{\mathrm{AIM}} = \sum \epsilon_p a_p^\dagger a_p + \sum \left(V_p^\sigma c_\sigma^\dagger a_{p\sigma} + h.c. \right) + U n_\uparrow n_\downarrow - \mu \left(n_\uparrow + n_\downarrow \right)$$

- Solution gives the Infinite Dimensions Hubbard Model Green Function

Lemma from Hohenberg and Kohn

The Ground State Density determines the Potential uniquely

$$n(r) \quad \longrightarrow \quad v(r)$$

The energy can be written in term of ground state density

$$E_{v(r)}[n(r)] = \int v(r)n(r)dr + F[n(r)]$$

$$F[n(r)] = T[n(r)] + \frac{1}{2}\int \frac{n(r)n(r^{'})}{|r - r^{'}|}drdr^{'} + E_{XC}[n(r)]$$

Hartree Approximation

Exchange Correlation

Self Consistent equation which generalizes the Hartree approximation

Kohn-Sham Equation

$$[-\frac{1}{2}\nabla^2 + v(r) + \int \frac{n(r^{'})}{|r - r^{'}|}dr^{'} + v_{XC}(r)]\phi_j(r) = \epsilon_j\phi_j(r)$$

$$E = \sum_j \epsilon_j - \frac{1}{2}\int \frac{n(r)n(r^{'})}{|r - r^{'}|}drdr^{'} - \int v_{XC}(d)n(r)dr - E_{XC}[n(r)]$$

Given the exchange correlation functional, the many body problem is mapped to a single body problem in a self-consistent field.

MuST (Multiple Scattering Theory) is an ab initio electronic structure calculation software suite, with petascale and beyond computing capability, for the first principles study of quantum phenomena in disordered materials.

Antisymmetric wavefunction for electrons

$$\psi(r_1, r_2, \cdots, r_N) = -\psi(r_2, r_1, \cdots, r_N)$$

Construct an antisymmetric many electrons wavefunction from single electron wavefunctions

$$\psi(r_1, r_2, \cdots) = Det\left[\phi_1(r_1)\phi_2(r_2)\cdots\phi_N(r_N)\right]$$

Independent electrons approximation, Hartree-Fock

$$\psi(r_1, r_2, \cdots) = Det\left[\phi_1(r_1)\phi_2(r_2)\cdots\phi_N(r_N)\right]$$

Schroedinger equation for each electron in an effective potential

$$\left[-\frac{\hbar^2}{2m}\nabla_i^2 + \sum_I V(R_I - r_i) + V_{Hartree-Fock}(r_i)\right]\phi_i(r_i) = \epsilon\phi_i(r_i)$$

Hatree Fock potential

$$V_{Hartree}(r_i) = \sum_j \int |\phi_j(r_j)|^2 \frac{1}{|r_i - r_j|} dr_j$$

Electron Density

$$n(r) = N \int |\Psi(r, r_2, \cdots, r_N)|^2 dr_2 \cdots dr_N$$

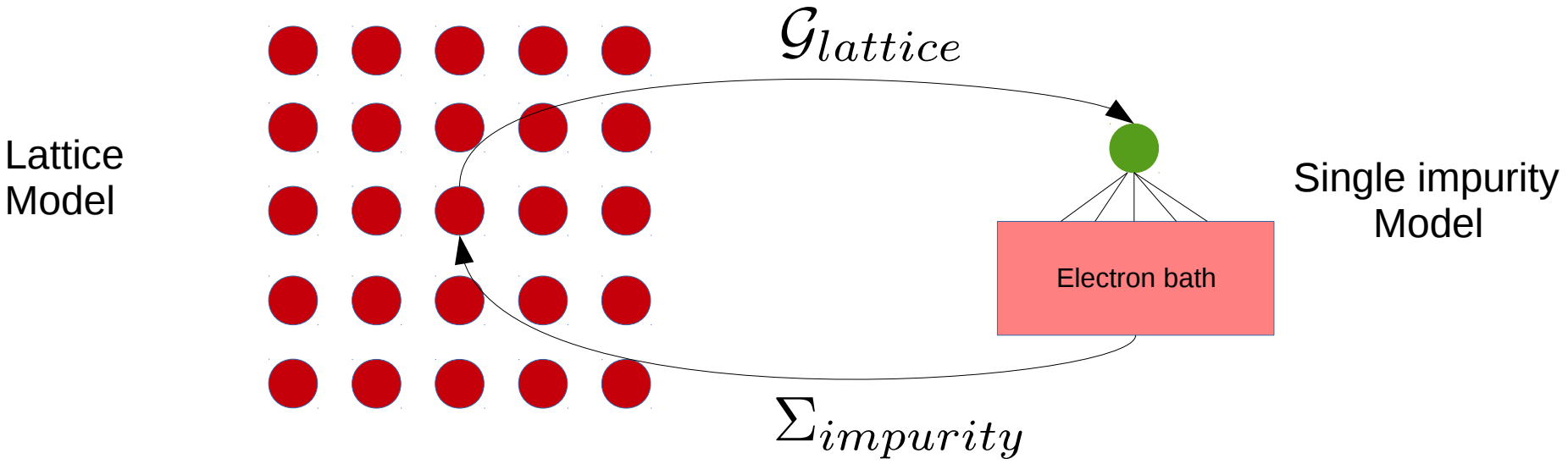
Ground state density determines the potential and the energy

$$\begin{aligned} \langle \Psi | H | \Psi \rangle &= \langle \Psi | T_e + V_{e-e} + v_{ext} | \Psi \rangle \\ &= \langle \Psi | T_e + V_{e-e} | \Psi \rangle + \int v_{ext} n \\ &= F(n) + \int v_{ext} n \end{aligned}$$

Functional of density

$$F(n) = T[n] + E_{Hartree}[n] + E_{XC}[n]$$

$$E = -\sum_i \frac{\hbar^2}{2m} \int \psi_i^*(r) \nabla_i^2 \psi_i(r) dr + E_{Hartree}[n] + E_{XC}[n] + \int v_{ext} n dr$$


Lattice Model
$\mathcal{G}_{lattice}$
Single impurity Model
Electron bath
$\Sigma_{impurity}$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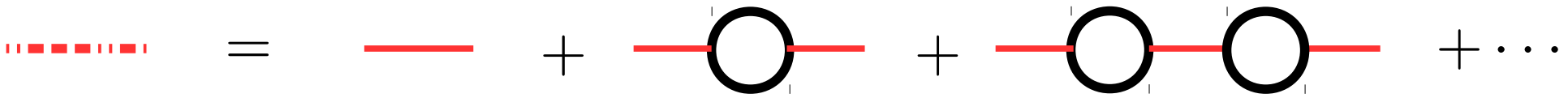
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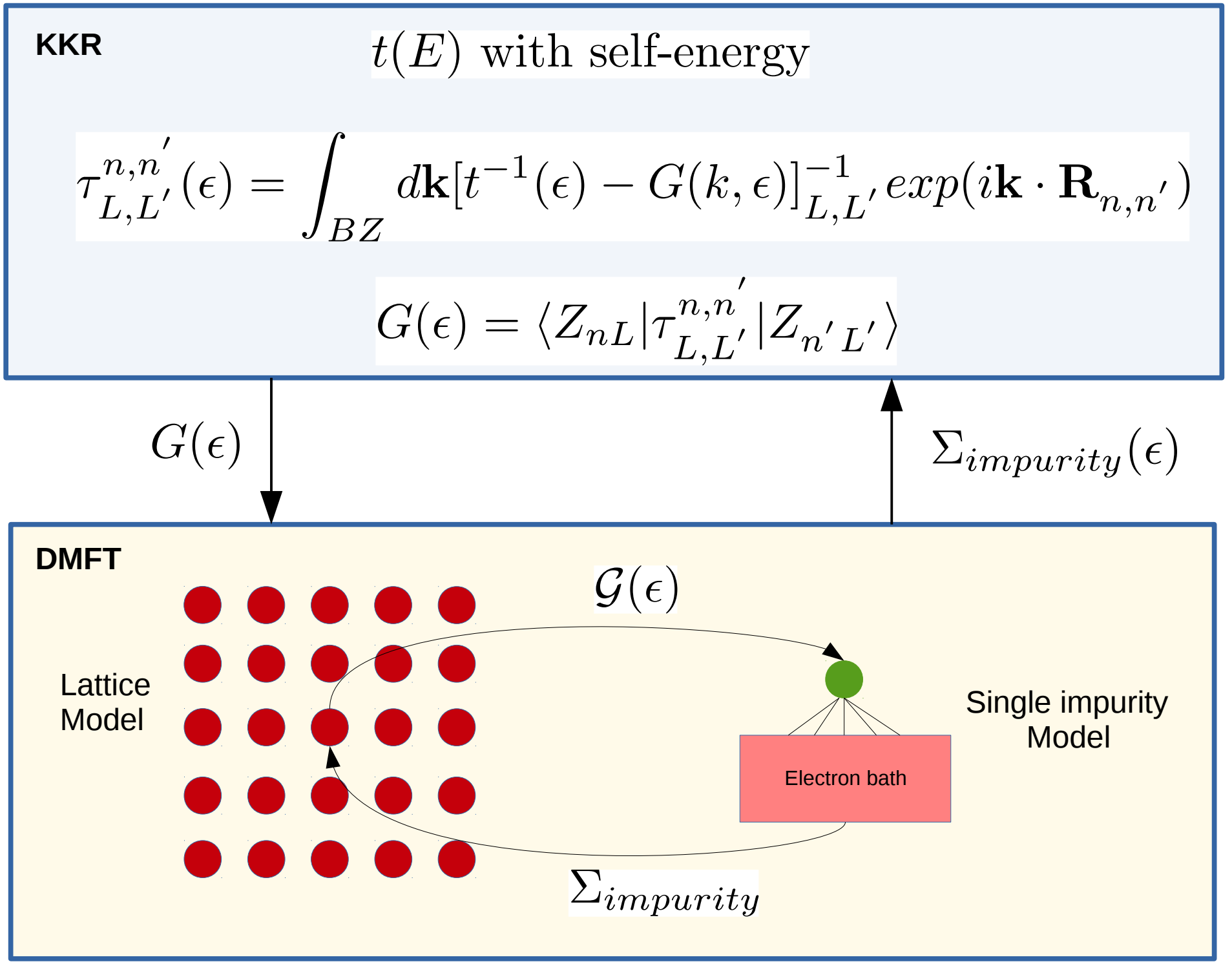
KKR
$t(E)$ with self-energy
$\tau^{n,n'}_{L,L'}(\epsilon) = \int_{BZ} d\mathbf{k}[t^{-1}(\epsilon) - G(k,\epsilon)]^{-1}_{L,L'} exp(i\mathbf{k}\cdot\mathbf{R}_{n,n'})$
$G(\epsilon) = \langle Z_{nL}|\tau^{n,n'}_{L,L'}|Z_{n'L'}\rangle$
$G(\epsilon)$
$\Sigma_{impurity}(\epsilon)$
DMFT
$\mathcal{G}(\epsilon)$
Lattice Model
Electron bath
Single impurity Model
$\Sigma_{impurity}$