Constrained RPA

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Motivation

Strongly correlated electrons are ...

- Hard to treat *ab initio*
- Should be described by a lattice model

$$H = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle,\sigma} c^{\dagger}_{\boldsymbol{i}\sigma} c_{\boldsymbol{j}\sigma} + \text{h.c.} + U \sum_{\boldsymbol{i}} n_{\boldsymbol{i}\uparrow} n_{\boldsymbol{i}\downarrow}. \tag{1}$$

But should all electrons be included?

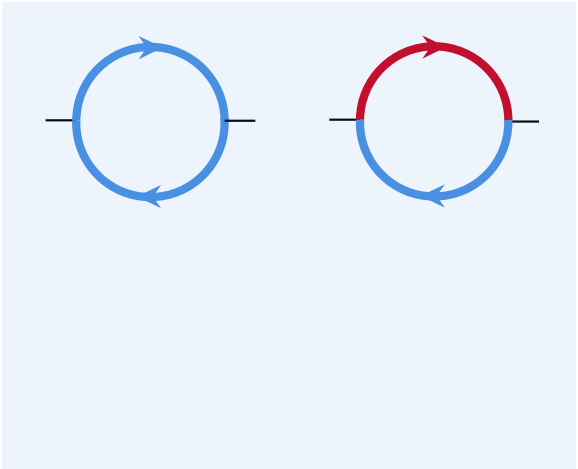
- d electron: correlated ones
- r electron: "trivial" ones

Diagrammatics

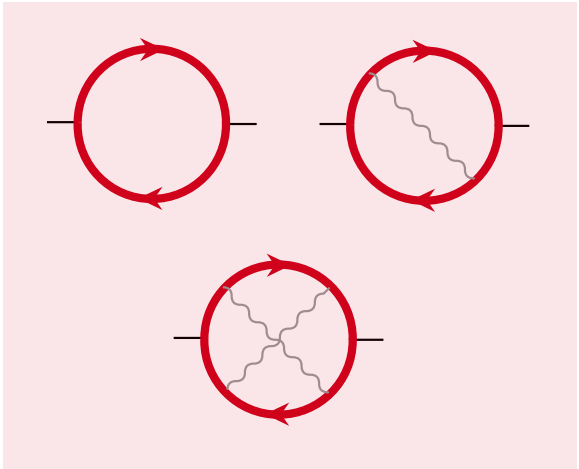
Screening by d and r = first screened by r and then d
Effective interaction:

$$W = (1 - vP)^{-1} v = (1 - W_r P_d)^{-1} W_r, \quad W_r = (1 - vP_r)^{-1} v, \qquad (2)$$

- where P_d is the polarization within d subspace,
- and $P_r = P - P_d$



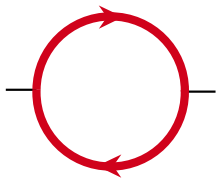
P_r
RPA works



P_d
RPA doesn't work

Diagrammatics

- P_d hard to obtain $\Rightarrow$ we left it to an effective interaction without doing resummation for it
- P_r can be done by `epsilon`
- But



  is not in P_r, or otherwise we have double counting
- That's what we call **constrained RPA (cRPA)**
- A program to calculate a single ring diagram is needed

Band part

In GW:

$$\begin{aligned} \varepsilon^{GW} &= \varepsilon^{0} + \Sigma^{\text{Hartree}} + \Sigma^{GW} \\ &= \underbrace{\varepsilon^{0} + \Sigma^{\text{Hartree}} + V^{\text{xc}}}_{\texttt{WFN}} + \underbrace{\Sigma^{GW}}_{\texttt{sigma}} - \underbrace{V^{\text{xc}}}_{\texttt{vxc.dat}} \end{aligned} \tag{3}$$

In the effective model ...

- We want ε^{0}
- So the same $-V^{\text{xc}}$ procedure is needed
- A problem to calculate a single ring diagram is needed.

Risks in accuracy

Uncontrolled approximation: does RPA work for