Karlsruhe Institute of Technology

Green functions and self-energy functionals

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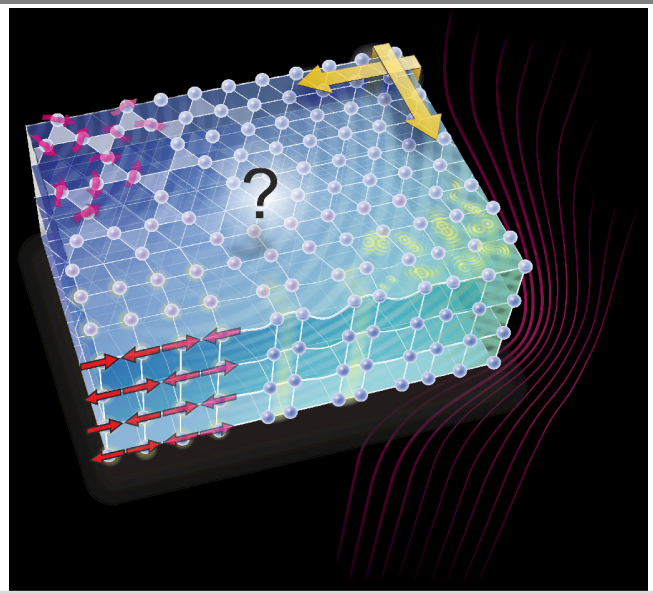
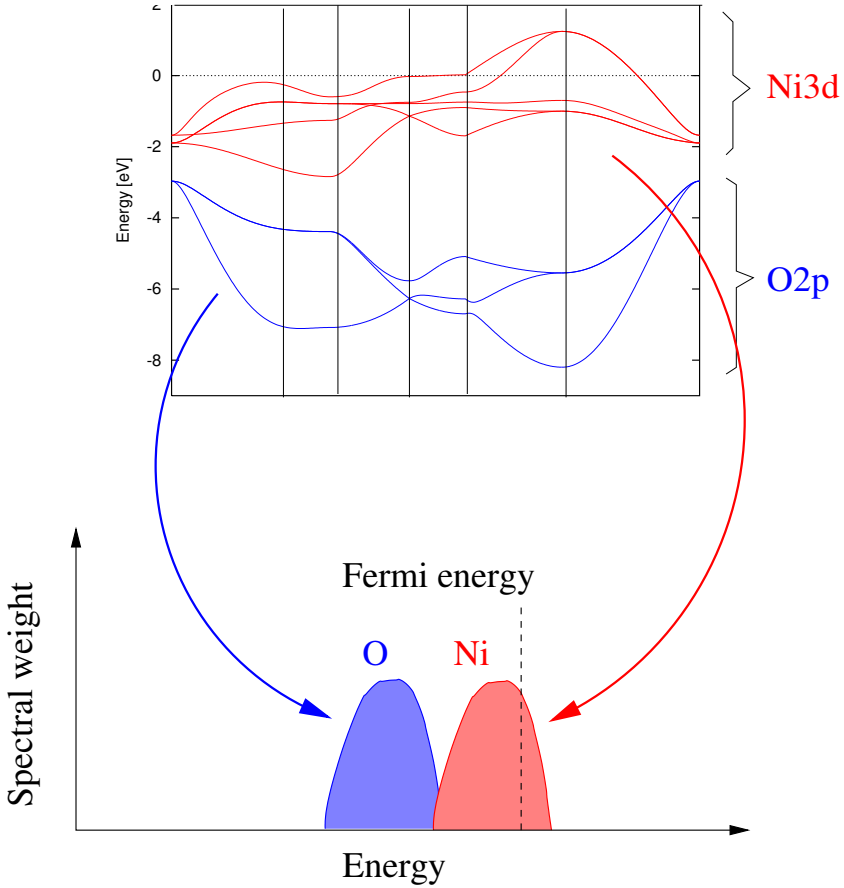
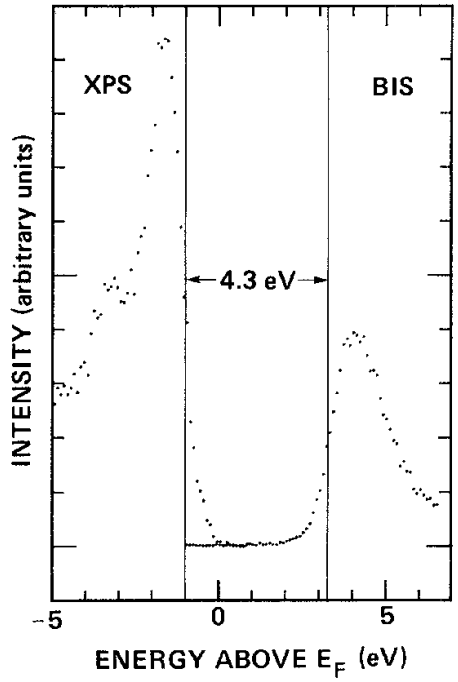


Prelude

DFT calculations do not describe correlated insulators such as NiO





G. A. Sawatzky and J. W. Allen
Phys. Rev. Lett. **53**, 2239 (1984).

Prelude

- We consider a Grand Canonical Ensemble at inverse temperature $\beta = 1/k_B T$ and chemical potential μ
- Let $\phi_\alpha(x)$ be a complete and orthonormal basis of single particle states

  - for example $\alpha = (n, \mathbf{k}, \sigma)$ or $\alpha = (\nu, \mathbf{R}_i, \sigma)$
- Define the corresponding Fermion operators $c_\alpha^\dagger$ and c_α
- The 'Grand Canonical Hamiltonian' $K = H - \mu N$ is $K = K_0 + K_1$ with

$$K_0 = \sum_{\alpha,\beta} \left(t_{\alpha,\beta} - \mu\, \delta_{\alpha,\beta}\right) c_\alpha^\dagger c_\beta, \qquad K_1 = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha,\beta,\delta,\gamma}\, c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$$

- We assume that we know all eigenstates $K\,|i\rangle = K_i\,|i\rangle$ - then

$$Z = \sum_i e^{-\beta K_i} \qquad \Omega = -\frac{1}{\beta} \log(Z) \qquad \langle O \rangle_{th} = \sum_i \frac{e^{-\beta K_i}}{Z} \langle i|O|i\rangle$$

The time-ordered imaginary time Green's function

Define the imaginary time Heisenberg operators (with $it \to \tau$) ...

$$c_\alpha(\tau) = e^{\tau \frac{K}{\hbar}}\, c_\alpha\, e^{-\tau \frac{K}{\hbar}} \qquad\qquad c^\dagger_\beta(\tau') = e^{\tau' \frac{K}{\hbar}}\, c^\dagger_\beta\, e^{-\tau' \frac{K}{\hbar}}$$

... and the time-ordered imaginary time Green's function

$$\begin{aligned}
G_{\alpha,\beta}(\tau,\tau') &= -\langle T\, c_\alpha(\tau)\, c^\dagger_\beta(\tau')\, \rangle_{th} \\
&= -\Theta(\tau-\tau')\langle\, c_\alpha(\tau)\, c^\dagger_\beta(\tau')\, \rangle_{th} + \Theta(\tau'-\tau)\langle\, c^\dagger_\beta(\tau')\, c_\alpha(\tau)\, \rangle_{th} \\
&= -\Theta(\tau-\tau') \sum_i \frac{e^{-\beta K_i}}{Z} \langle i|c_\alpha(\tau) c^\dagger_\beta(\tau')|i\rangle \\
&\qquad + \Theta(\tau'-\tau) \sum_i \frac{e^{-\beta K_i}}{Z} \langle i|c^\dagger_\beta(\tau') c_\alpha(\tau)|i\rangle
\end{aligned}$$

The time-ordered imaginary time Green's function, cont'd

$$
\begin{aligned}
G_{\alpha,\beta}(\tau,\tau') &= -\Theta(\tau-\tau')\sum_i \frac{e^{-\beta K_i}}{Z}\,\langle i|c_\alpha(\tau)c_\beta^\dagger(\tau')|i\rangle \\
&\quad + \Theta(\tau'-\tau)\sum_i \frac{e^{-\beta K_i}}{Z}\,\langle i|c_\beta^\dagger(\tau')c_\alpha(\tau)|i\rangle \\
&= -\Theta(\tau-\tau')\sum_j\sum_i \frac{e^{-\beta K_i}}{Z}\,\langle i|c_\alpha(\tau)|j\rangle\,\langle j|c_\beta^\dagger(\tau')|i\rangle \\
&\quad + \Theta(\tau'-\tau)\sum_j\sum_i \frac{e^{-\beta K_i}}{Z}\,\langle i|c_\beta^\dagger(\tau')|j\rangle\,\langle j|c_\alpha(\tau)|i\rangle \\
&= -\Theta(\tau-\tau')\sum_{i,j} \frac{e^{-\beta K_i}}{Z}\,\langle i|e^{\tau\frac{K}{\hbar}}\,c_\alpha\,e^{-\tau\frac{K}{\hbar}}|j\rangle\,\langle j|e^{\tau'\frac{K}{\hbar}}\,c_\beta^\dagger\,e^{-\tau'\frac{K}{\hbar}}|i\rangle \\
&\quad + \Theta(\tau'-\tau)\sum_{i,j} \frac{e^{-\beta K_i}}{Z}\,\langle i|e^{\tau'\frac{K}{\hbar}}\,c_\beta^\dagger\,e^{-\tau'\frac{K}{\hbar}}|j\rangle\,\langle j|e^{\tau\frac{K}{\hbar}}\,c_\alpha\,e^{-\tau\frac{K}{\hbar}}|i\rangle
\end{aligned}
$$

The time-ordered imaginary time Green's function, cont'd

$$G_{\alpha,\beta}(\tau,\tau') = -\Theta(\tau-\tau')\sum_{i,j}\frac{e^{-\beta K_i}}{Z}\langle i|e^{\tau\frac{K}{\hbar}}\,c_\alpha\,e^{-\tau\frac{K}{\hbar}}|j\rangle\,\langle j|e^{\tau'\frac{K}{\hbar}}\,c_\beta^\dagger\,e^{-\tau'\frac{K}{\hbar}}|i\rangle$$

$$+\Theta(\tau'-\tau)\sum_{i,j}\frac{e^{-\beta K_i}}{Z}\langle i|e^{\tau'\frac{K}{\hbar}}\,c_\beta^\dagger\,e^{-\tau'\frac{K}{\hbar}}|j\rangle\,\langle j|e^{\tau\frac{K}{\hbar}}\,c_\alpha\,e^{-\tau\frac{K}{\hbar}}|i\rangle$$

$$\langle i|e^{\tau\frac{K}{\hbar}}\,c_\alpha\,e^{-\tau\frac{K}{\hbar}}|j\rangle\langle j|e^{\tau'\frac{K}{\hbar}}\,c_\beta^\dagger\,e^{-\tau'\frac{K}{\hbar}}|i\rangle = e^{\tau\frac{K_i-K_j}{\hbar}}\langle i|c_\alpha|j\rangle\,e^{\tau'\frac{K_j-K_i}{\hbar}}\langle j|c_\beta^\dagger|i\rangle$$

$$= e^{(\tau-\tau')\frac{K_i-K_j}{\hbar}}\langle i|c_\alpha|j\rangle\,\langle j|c_\beta^\dagger|i\rangle$$

$$G_{\alpha,\beta}(\tau,\tau') = -\Theta(\tau-\tau')\sum_{i,j}\frac{e^{-\beta K_i}}{Z}\,e^{(\tau-\tau')\frac{K_i-K_j}{\hbar}}\,\langle i|c_\alpha|j\rangle\,\langle j|c_\beta^\dagger|i\rangle$$

$$+\Theta(\tau'-\tau)\sum_{i,j}\frac{e^{-\beta K_i}}{Z}\,e^{(\tau-\tau')\frac{K_j-K_i}{\hbar}}\,\langle i|c_\beta^\dagger|j\rangle\,\langle j|c_\alpha|i\rangle$$

Fourier transform

$$G_{\alpha,\beta}(\tau) = -\Theta(\tau) \sum_{i,j} \frac{e^{-\beta K_i}}{Z} e^{\tau \frac{K_i - K_j}{\hbar}} \langle i|c_\alpha|j\rangle \langle j|c_\beta^\dagger|i\rangle + \Theta(-\tau) \sum_{i,j} \frac{e^{-\beta K_i}}{Z} e^{\tau \frac{K_j - K_i}{\hbar}} \langle i|c_\beta^\dagger|j\rangle \langle j|c_\alpha|i\rangle$$

- Well defined only for $\tau \in [-\hbar\beta, \hbar\beta] \Rightarrow$ Fourier frequencies $\omega_n = n \frac{2\pi}{2\hbar\beta} = n \frac{\pi}{\hbar\beta}$

$$G(\tau) \propto \sum_{n=-\infty}^{\infty} e^{-i\omega_n \tau} G(i\omega_n)$$

- Boundary condition: $G(\tau + \hbar\beta) = -G(\tau) \Rightarrow n = 2\nu + 1$

$$G(\tau) = \frac{1}{\hbar\beta} \sum_{\nu=-\infty}^{\infty} e^{-i\omega_\nu \tau} G(i\omega_\nu), \qquad G(i\omega_\nu) = \int_0^{\hbar\beta} d\tau\, e^{i\omega_\nu \tau} G(\tau)$$

- Fermionic Matsubara frequencies $\omega_\nu = \frac{(2\nu+1)\pi}{\hbar\beta}$

We recall the Green's function ...

$$G_{\alpha,\beta}(\tau) \;=\; -\Theta(\tau)\sum_{i,j}\frac{e^{-\beta K_i}}{Z}\,e^{\tau\frac{K_i-K_j}{\hbar}}\,\langle i|c_\alpha|j\rangle\,\langle j|c_\beta^\dagger|i\rangle + \Theta(-\tau)\ldots$$

... and evaluate its Fourier transform

$$G_{\alpha,\beta}(i\omega_\nu) \;=\; \int_0^{\hbar\beta} d\tau\; e^{i\omega_\nu\tau}\; G_{\alpha,\beta}(\tau)$$

$$e^{-\beta K_i}\int_0^{\hbar\beta} d\tau\; e^{\tau(i\omega_\nu+\frac{K_i-K_j}{\hbar})} = e^{-\beta K_i}\;\left.\frac{e^{\tau(i\omega_\nu+\frac{K_i-K_j}{\hbar})}}{i\omega_\nu+\frac{K_i-K_j}{\hbar}}\right|_0^{\hbar\beta} = -\frac{e^{-\beta K_i}+e^{-\beta K_j}}{i\omega_\nu-\frac{K_j-K_i}{\hbar}}$$

In this way we obtain the Lehmann representation:

$$G_{\alpha,\beta}(i\omega_\nu) \;=\; \sum_{i,j}\frac{e^{-\beta K_i}+e^{-\beta K_j}}{Z}\;\frac{\langle i|c_\alpha|j\rangle\,\langle j|c_\beta^\dagger|i\rangle}{i\omega_\nu-\frac{K_j-K_i}{\hbar}}$$

Real time Green's function

Now consider the real-time Heisenberg operators ...

$$c_\alpha(t) = e^{it\frac{K}{\hbar}}\, c_\alpha\, e^{-it\frac{K}{\hbar}} \qquad c^\dagger_\beta(it') = e^{it'\frac{K}{\hbar}}\, c^\dagger_\beta\, e^{-it'\frac{K}{\hbar}}$$

... and the retarded real-time Green's function

$$\begin{aligned} G^R_{\alpha,\beta}(t,t') &= -i\,\Theta(t-t')\,\langle\,\left\{c_\alpha(t), c^\dagger_\beta(t')\right\}\,\rangle_{th} \\ &= -i\,\Theta(t-t')\,\left(\,\langle\, c_\alpha(t)c^\dagger_\beta(t')\,\rangle_{th} + \langle c^\dagger_\beta(t')c_\alpha(t)\,\rangle_{th}\,\right) \end{aligned}$$

Now compare with the time-ordered imaginary time Green's function

$$G_{\alpha,\beta}(\tau,\tau') = -\Theta(\tau-\tau')\langle\, c_\alpha(\tau)\, c^\dagger_\beta(\tau')\,\rangle_{th} + \Theta(\tau'-\tau)\langle\, c^\dagger_\beta(\tau')\, c_\alpha(\tau)\,\rangle_{th}$$

- $\tau \to it$ and $\pm\Theta\left(\pm(\tau'-\tau)\right) \to -i\,\Theta(t-t')$

Fourier transform

$$G^R_{\alpha,\beta}(t) \quad = \quad -i\,\Theta(t)\sum_{i,j}\frac{e^{-\beta K_i}+e^{-\beta K_j}}{Z}\,e^{-it\frac{K_j-K_i}{\hbar}}\,\langle i|c_\alpha|j\rangle\,\langle j|c^\dagger_\beta|i\rangle$$

- No limitation on t - we seek the conventional Fourier transform

$$G^R_{\alpha,\beta}(t) \quad = \quad \frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\; e^{-i\omega t}\; G^R_{\alpha,\beta}(\omega)$$

- We use the formula (Appendix A of my notes)

$$-i\Theta(t)e^{-iEt} \quad = \quad \lim_{\eta\to 0^+}\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\; e^{-i\omega t}\;\frac{1}{\omega-E+i\eta}$$

$$\Rightarrow\; G^R_{\alpha,\beta}(\omega) \quad = \quad \lim_{\eta\to 0^+}\sum_{i,j}\frac{e^{-\beta K_i}+\;e^{-\beta K_j}}{Z}\;\frac{\langle i|c_\alpha|j\rangle\,\langle j|c^\dagger_\beta|i\rangle}{\omega-\frac{K_j-K_i}{\hbar}+i\eta}$$

Now compare:

$$G_{\alpha,\beta}(i\omega_\nu) = \sum_{i,j} \frac{e^{-\beta K_i} + e^{-\beta K_j}}{Z} \frac{\langle i|c_\alpha|j\rangle \langle j|c_\beta^\dagger|i\rangle}{i\omega_\nu - \frac{K_j - K_i}{\hbar}}$$

$$G^R_{\alpha,\beta}(\omega) = \lim_{\eta\to 0^+} \sum_{i,j} \frac{e^{-\beta K_i} + e^{-\beta K_j}}{Z} \frac{\langle i|c_\alpha|j\rangle \langle j|c_\beta^\dagger|i\rangle}{\omega + i\eta - \frac{K_j - K_i}{\hbar}}$$

- There is one function $G_{\alpha,\beta}(z)$ of the complex variable z - called 'the' Green's function - which gives $G_{\alpha,\beta}(i\omega_\nu)$ when evaluated at the Matsubara frequencies and $G^R_{\alpha,\beta}(\omega)$ when evaluated at a line infinitesimally above the real axis

$$G_{\alpha,\beta}(z) = \sum_{i,j} \frac{e^{-\beta K_i} + e^{-\beta K_j}}{Z} \frac{\langle i|c_\alpha|j\rangle \langle j|c_\beta^\dagger|i\rangle}{z - \frac{K_j - K_i}{\hbar}}$$

Why is that important?

- The imaginary-time Green's function is better to handle mathematically
- It can be written as a Grassmann functional integral and expanded into Feynman diagrams whereas the real-time Green's function cannot
- Therefore a procedure that is followed in hundreds of papers is as follows:
- Evaluate an approximate $G(i\omega_\nu)$ e.g. by Feynman diagram expansion and some trick e.g. summation of subclass of diagrams
- Then simply replace $G(i\omega_\nu) \rightarrow G(\omega + i\eta)$ to obtain an approximate real-time Green's function

Rewriting G

$$
\begin{aligned}
G_{\alpha,\beta}(z) &= \sum_{i,j} \frac{e^{-\beta K_i} + e^{-\beta K_j}}{Z} \frac{\langle i|c_\alpha|j\rangle \langle j|c_\beta^\dagger|i\rangle}{z - \frac{K_j - K_i}{\hbar}} \\
&= \sum_{i,j} \frac{e^{-\beta K_i}}{Z} \frac{\langle i|c_\alpha|j\rangle \langle j|c_\beta^\dagger|i\rangle}{z - \frac{K_j - K_i}{\hbar}} + \sum_{i,j} \frac{e^{-\beta K_j}}{Z} \frac{\langle i|c_\alpha|j\rangle \langle j|c_\beta^\dagger|i\rangle}{z - \frac{K_j - K_i}{\hbar}} \\
&= \sum_{i,j} \frac{e^{-\beta K_i}}{Z} \frac{\langle i|c_\alpha|j\rangle \langle j|c_\beta^\dagger|i\rangle}{z - \frac{K_j - K_i}{\hbar}} + \sum_{i,j} \frac{e^{-\beta K_i}}{Z} \frac{\langle i|c_\beta^\dagger|j\rangle \langle j|c_\alpha|i\rangle}{z + \frac{K_j - K_i}{\hbar}}
\end{aligned}
$$

Physical interpretation

- We assume $c_\alpha = c_{\mathbf{k},\sigma}$, $c_\beta^\dagger = c_{\mathbf{k},\sigma}^\dagger$
- The expression for 'the' Green's function becomes

$$G_{\mathbf{k},\sigma}(z) = \sum_{i,j} \frac{e^{-\beta K_i}}{Z} \left[\frac{\langle i|c_{\mathbf{k},\sigma}|j\rangle \langle j|c_{\mathbf{k},\sigma}^\dagger|i\rangle}{z - \frac{K_j - K_i}{\hbar}} + \frac{\langle i|c_{\mathbf{k},\sigma}^\dagger|j\rangle \langle j|c_{\mathbf{k},\sigma}|i\rangle}{z + \frac{K_j - K_i}{\hbar}} \right]$$

- $|j\rangle$ has one electron less than $|i\rangle$ - $|j\rangle$ has one electron more than $|i\rangle$
- $K_j - K_i$ is the energy needed to remove/add an electron with wave vector **k**
- Assume $K = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu)\, c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma}$
- Then $K_j = K_i \pm (\epsilon_{\mathbf{k}} - \mu) \Rightarrow K_j - K_i = \pm(\epsilon_{\mathbf{k}} - \mu)$
- $G_{\mathbf{k},\sigma}(z)$ has poles on the real z-axis - the dispersion with **k** gives the band structure observed inphotoemission/inverse photoemission

Noninteracting case

$$G_{\mathbf{k},\sigma}(z) = \sum_{i,j} \frac{e^{-\beta K_i}}{Z} \left[\frac{\langle i|c_{\mathbf{k},\sigma}|j\rangle\langle j|c^\dagger_{\mathbf{k},\sigma}|i\rangle}{z - \frac{K_j - K_i}{\hbar}} + \frac{\langle i|c^\dagger_{\mathbf{k},\sigma}|j\rangle\langle j|c_{\mathbf{k},\sigma}|i\rangle}{z + \frac{K_j - K_i}{\hbar}} \right]$$

Assume $K = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu)\, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$

- Then $K_j = K_i \pm (\epsilon_{\mathbf{k}} - \mu) \Rightarrow K_j - K_i = \pm(\epsilon_{\mathbf{k}} - \mu)$ - independent of $|j\rangle$

$$G_{\mathbf{k},\sigma}(z) = \sum_i \frac{e^{-\beta K_i}}{Z} \left[\frac{\langle i|c_{\mathbf{k},\sigma}c^\dagger_{\mathbf{k},\sigma}|i\rangle}{z - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar}} + \frac{\langle i|c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}|i\rangle}{z - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar}} \right]$$

$$= \frac{1 - f_{\mathbf{k},\sigma}}{z - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar}} + \frac{f_{\mathbf{k},\sigma}}{z - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar}}$$

$$= \frac{1}{z - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar}}$$

Noninteracting case

- For noninteracting 'band electrons' ...

$$K_0 = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu)\; c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \quad \Rightarrow \quad G_{0,\mathbf{k},\sigma}(z) = \frac{1}{z - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar}}$$

- The generalization to an arbitrary noninteracting Hamiltonian is ...

$$K_0 = \sum_{\alpha,\beta} (t_{\alpha,\beta} - \mu\; \delta_{\alpha,\beta})\; c^{\dagger}_{\alpha} c_{\beta} \quad \Rightarrow \quad \mathbf{G}_0(z) = \left(z - \frac{\mathbf{t} - \mu}{\hbar} \right)^{-1}$$

... where $\mathbf{G}_0(z)$ and $\mathbf{t}$ are matrices of dimension $2n_{orb} \times 2n_{orb}$

Check: Set $t_{\alpha,\beta} = \epsilon_{\mathbf{k}}\; \delta_{\alpha,\beta}$

The self energy

- For a noninteracting Hamiltonian ...

$$K_0 = \sum_{\alpha,\beta} \left(t_{\alpha,\beta} - \mu\ \delta_{\alpha,\beta}\right)\ c_\alpha^\dagger c_\beta \quad \Rightarrow \quad \mathbf{G}_0(z) = \left(z - \frac{\mathbf{t} - \mu}{\hbar} \right)^{-1}$$

- For an interacting Hamiltonian ...

$$K = \sum_{\alpha,\beta} \left(t_{\alpha,\beta} - \mu\ \delta_{\alpha,\beta}\right)\ c_\alpha^\dagger c_\beta + \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha,\beta,\delta,\gamma}\ c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$$

... we define the self energy $\Sigma(z)$ by the Dyson equation

$$\mathbf{G}(z) = \left(z - \frac{\mathbf{t} - \mu}{\hbar} - \Sigma(z) \right)^{-1} = \left(\mathbf{G}_0^{-1}(z) - \Sigma(z) \right)^{-1}$$

$$\mathbf{G}^{-1}(z) = z - \frac{\mathbf{t} - \mu}{\hbar} - \Sigma(z) = \mathbf{G}_0^{-1}(z) - \Sigma(z)$$

Interacting band structure

- For ‘band electrons’ we have

$$G^{-1}_{\mathbf{k},\sigma}(z) \quad = \quad z - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar} - \Sigma_{\mathbf{k}}(z)$$

- But recall:
- $G_{\mathbf{k},\sigma}(z)$ has poles on the real z-axis - the dispersion with $\mathbf{k}$ gives the band structure observed inphotoemission/inverse photoemission
- However, a pole of $G_{\mathbf{k},\sigma}(z)$ means $G^{-1}_{\mathbf{k},\sigma}(z) = 0$
- The equation for the interacting band dispersion $E_{\mathbf{k}} = \hbar\omega_{\mathbf{k}}$ therefore is

$$\omega_{\mathbf{k}} - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar} - \Sigma_{\mathbf{k}}(\omega_{\mathbf{k}}) \quad = \quad 0$$

For simplicity we drop μ, omit $\mathbf{k}$ and set $\hbar = 1$

$$\omega - \epsilon - \Sigma(\omega) = 0$$

We seek solutions of $\omega - \epsilon - \Sigma(\omega) = 0$

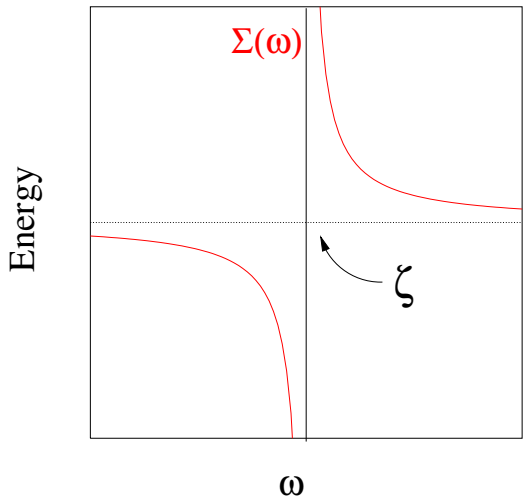
$\Sigma(\omega)$ has the form (see my notes)

$$\Sigma(\omega) = V_{HF} + \sum_i \frac{\sigma_i}{\omega - \zeta_i}$$

To see the implications of this let us consider just a single pole:

$$\Sigma(\omega) = \frac{\sigma}{\omega - \zeta}$$

The equation for poles of the Green's function is: $\omega - \epsilon_{\mathbf{k}} = \Sigma(\omega)$



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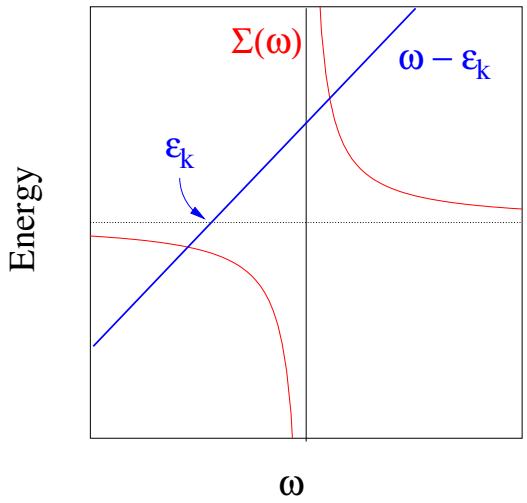

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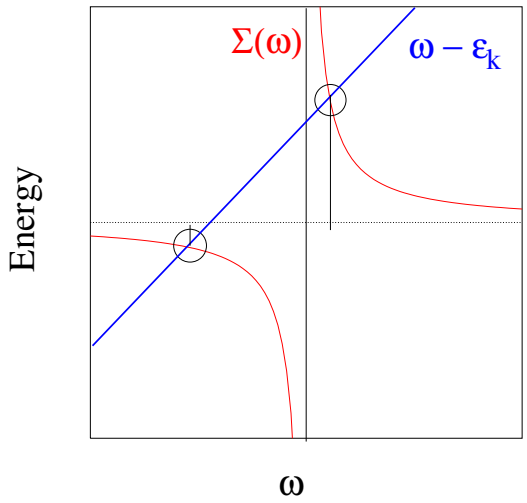

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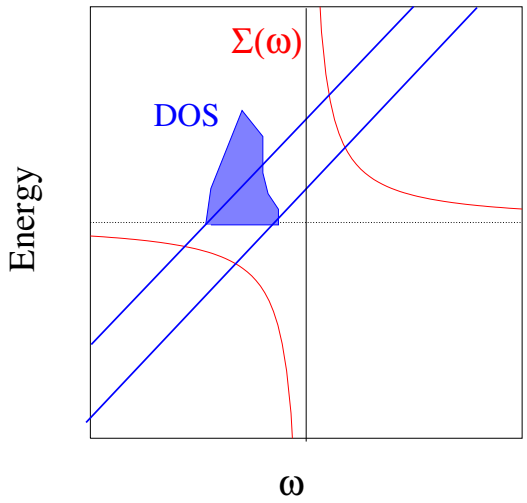

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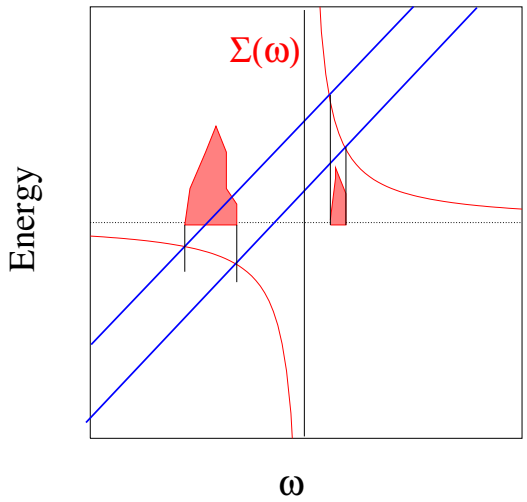

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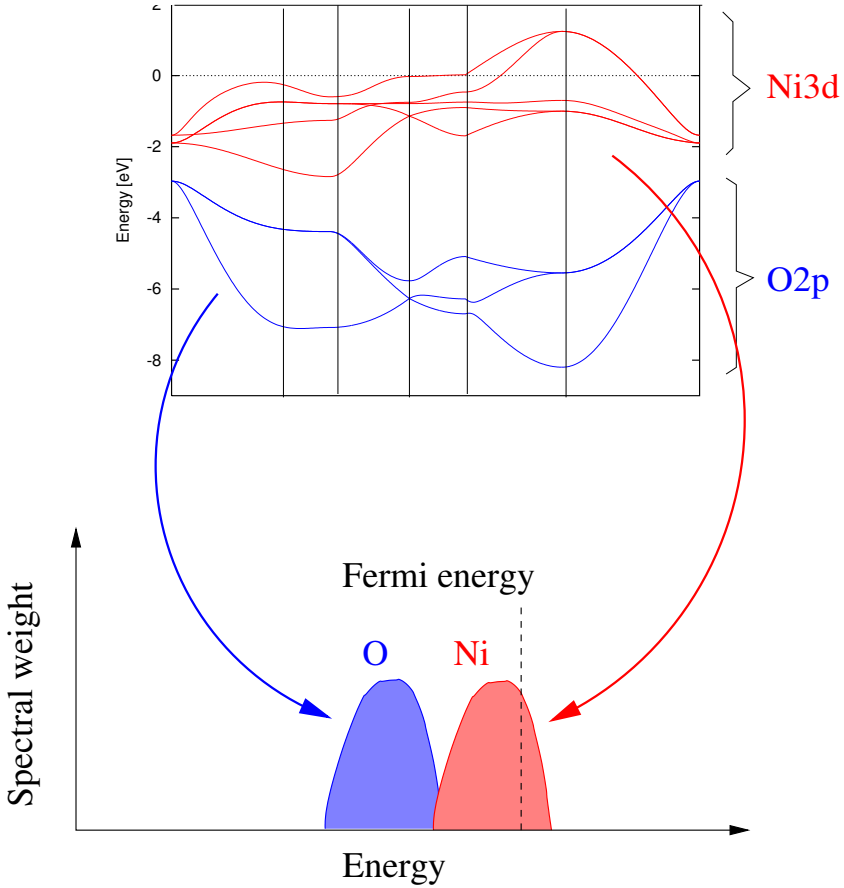

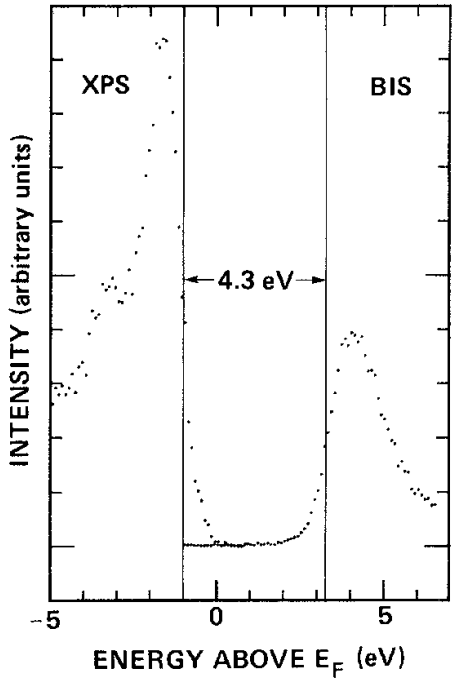

G. A. Sawatzky and J. W. Allen
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Crash course in Grassmann variables

- Grassmann variables are objects - we write them as ϕ_i or ϕ_j^*, where i and j distinguish different Grassman variables - which anticommute

$$\phi_i^* \phi_j^* = -\phi_j^* \phi_i^* \qquad \phi_i \phi_j^* = -\phi_j^* \phi_i, \qquad \phi_i \phi_j = -\phi_j \phi_i.$$

- The asterisk * is part of the name of the Grassmann variable
- $\phi_i^* \phi_i^* = -\phi_i^* \phi_i^* = 0$ - the square of any Grassmann variable is zero
- A Grassmann algebra consists of all combinations of nonvanishing products of the 'Grassmann basis', e.g. with basis ϕ and ϕ^*

$$a_0 + a_1 \phi + a_2 \phi^* + a_3 \phi \phi^*$$

- The key property of Grassmann variables is the rule for 'integration'

$$\int d\phi \, \phi = 1, \qquad \int d\phi \, 1 = 0$$

Crash course in Grassmann variables

- Functions of Grassmann variables are defined via the power series expansion

$$\begin{aligned} exp(a_1\phi + a_2\phi^* + a_3\phi^*\phi) &= 1 + (a_1\phi + a_2\phi^* + a_3\phi^*\phi) + \frac{1}{2!}a_1 a_2(\phi\phi^* + \phi^*\phi) \\ &= 1 + (a_1\phi + a_2\phi^* + a_3\phi^*\phi) \end{aligned}$$

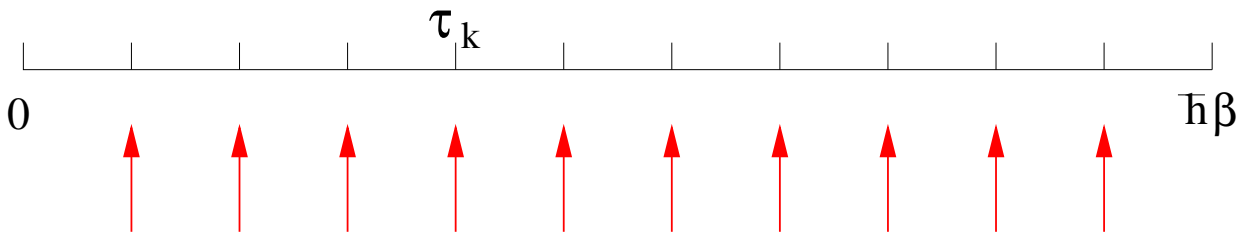
Therefore

$$\begin{aligned} \int d\phi^*\, d\phi\, exp(a_1\phi + a_2\phi^* + a_3\phi^*\phi) &= a_3 \int d\phi^*\, d\phi\, \phi^*\, \phi \\ &= -a_3 \int d\phi^*\, d\phi\, \phi\, \phi^* \\ &= -a_3 \int d\phi^*\, \phi^* = -a_3 \end{aligned}$$

Crash course in functional integrals

- Divide $[0, \hbar\beta]$ into M intervals of length $\epsilon = \hbar\beta / M$ with $M \to \infty$

$$Z = \mathrm{tr}\, e^{-\beta K} = \mathrm{tr}\, e^{-\hbar\beta \frac{K}{\hbar}} = \mathrm{tr}\, \left(e^{-\epsilon \frac{K}{\hbar}} \right)^M$$



- At each grid point $\tau_k = k \cdot \epsilon$ insert resolution of unity
- Here in terms of Fermion coherent states $|\Phi_k\rangle\langle\Phi_k|$

$$c_\gamma |\Phi_k\rangle\langle\Phi_k| = \phi_{\gamma,k} |\Phi_k\rangle\langle\Phi_k|$$

$$|\Phi_k\rangle\langle\Phi_k| c_\gamma^\dagger = |\Phi_k\rangle\langle\Phi_k| \phi_{\gamma,k}^*$$

Crash course in functional integrals

The Hamiltonian was

$$K = \sum_{\alpha,\beta} \left(t_{\alpha,\beta} - \mu \, \delta_{\alpha,\beta} \right) c_\alpha^\dagger c_\beta + \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha,\beta,\delta,\gamma} \, c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$$

Then, since $\epsilon = \frac{\hbar\beta}{M} \to 0$

$$\begin{aligned}
|\Phi_k\rangle\langle\Phi_k| e^{\epsilon \frac{K}{\hbar}} |\Phi_{k-1}\rangle\langle\Phi_{k-1}| &= |\Phi_k\rangle\langle\Phi_k| \left(1 + \epsilon \, \frac{K(c^\dagger, c)}{\hbar}\right) |\Phi_{k-1}\rangle\langle\Phi_{k-1}| + 0(\epsilon^2) \\
&= |\Phi_k\rangle\langle\Phi_k| \left(1 + \epsilon \, \frac{K(\phi_k^*, \phi_{k-1})}{\hbar}\right) |\Phi_{k-1}\rangle\langle\Phi_{k-1}| + \ldots \\
&= |\Phi_k\rangle\langle\Phi_k| e^{\epsilon \, \frac{K(\phi_k^*, \phi_{k-1})}{\hbar}} |\Phi_{k-1}\rangle\langle\Phi_{k-1}| + 0(\epsilon^2)
\end{aligned}$$

- Analogous to derivation of the Feynman path integral for $U(0,t) = e^{-\frac{it}{\hbar}H}$

Grassmann variable representation of Z

- Let $[0, \hbar\beta]$ be divided into M intervals of length $\epsilon = \hbar\beta / M$
- Define imaginary time grid points $\tau_k = k \cdot \epsilon$, $k = 1 \ldots M$
- For each grid point τ_k introduce Grassmann variables $\phi^*_{\gamma,k}$ and $\phi_{\gamma,k}$
- γ is the 'compound index' on Fermion operators $c^\dagger_\gamma$ and c_γ

$$Z = \lim_{M\to\infty} \prod_{k=1}^{M} \prod_{\gamma} \int d\phi^*_{\gamma,k}\, d\phi_{\gamma,k}\, e^{-S_M(\phi^*,\phi)}$$

$$S_M(\phi^*,\phi) = \sum_{k=1}^{M} \epsilon \left[\sum_{\gamma} \phi^*_{\gamma,k} \frac{\phi_{\gamma,k} - \phi_{\gamma,k-1}}{\epsilon} + \frac{1}{\hbar} K(\phi^*_k, \phi_{k-1}) \right]$$

- $K(\phi^*_k, \phi_{k-1})$: Grand Canonical Hamiltonian with $c^\dagger_\gamma \to \phi^*_{\gamma,k}$ and $c_\gamma \to \phi_{\gamma,k-1}$
- This indeed reproduces Z for noninteracting Fermions, see my notes

Grassman variable representation of Z

Recall

$$S(\phi^*,\phi) \quad = \quad \lim_{M\to\infty} \sum_{k=1}^{M} \epsilon \left[\sum_{\gamma} \phi^*_{\gamma,k} \, \frac{\phi_{\gamma,k} - \phi_{\gamma,k-1}}{\epsilon} + \frac{1}{\hbar} K(\phi^*_k, \phi_{k-1}) \right]$$

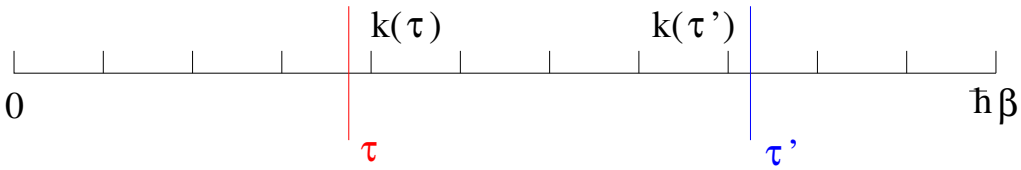
If we treat the Grassmann variables as 'numbers' and recall $\epsilon = \frac{\hbar\beta}{M}$

$$\Rightarrow S \quad \rightarrow \quad \int_0^{\hbar\beta} d\tau \left(\sum_{\gamma} \phi^*_{\gamma} \, \frac{\partial \phi_{\gamma}}{\partial \tau} + \frac{1}{\hbar} K(\phi^*, \phi) \right)$$

S is called the action associated with the Hamiltonian K

Green's function as a functional integral

- The imaginary time Green's function can also be rewritten



$$G_{\alpha,\beta}(\tau,\tau') = -\langle T\, c_\alpha(\tau)\, c^\dagger_\beta(\tau')\,\rangle_{th}$$

$$= -\lim_{M\to\infty} \frac{\prod_{k=1}^{M}\prod_\gamma \int d\phi^*_{\gamma,k}\, d\phi_{\gamma,k}\, \phi_{\alpha,k(\tau)}\phi^*{}_{\beta,k(\tau')}\, e^{-S_M(\phi^*,\phi)}}{\prod_{k=1}^{M}\prod_\gamma \int d\phi^*_{\gamma,k}\, d\phi_{\gamma,k}\, e^{-S_M(\phi^*,\phi)}}$$

- In order to take the limit $M \to \infty$ easily we switch to Fourier transformed Grassmann variables

Fourier transform of S

- Define the Fourier transformed Grassmann variables (with $\omega_\nu = \frac{(2\nu+1)\pi}{\hbar\beta}$)

$$\tilde{\phi}^*_{\gamma,\nu} = \frac{1}{\sqrt{M}} \sum_{k=1}^{M} e^{-i\,\omega_\nu \tau_k}\, \phi^*_{\gamma,k}, \qquad \tilde{\phi}_{\gamma,\nu} = \frac{1}{\sqrt{M}} \sum_{k=1}^{M} e^{i\,\omega_\nu \tau_k}\, \phi_{\gamma,k}$$

- This is easily reverted

$$\phi^*_{\gamma,k} = \frac{1}{\sqrt{M}} \sum_{\nu=-\frac{M}{2}+1}^{\frac{M}{2}} e^{i\omega_\nu \tau_k}\, \tilde{\phi}^*_{\gamma,\nu}, \qquad \phi_{\gamma,k} = \frac{1}{\sqrt{M}} \sum_{\nu=-\frac{M}{2}+1}^{\frac{M}{2}} e^{-i\omega_\nu \tau_k}\, \tilde{\phi}_{\gamma,\nu}.$$

- The transformation $\phi^*_{\gamma,k} \to \tilde{\phi}^*_{\gamma,\nu}$ is unitary $\Rightarrow$ the Jacobian is unity
- The limit $M \to \infty$ is trivial to take

Fourier transform of S

- After some algebra (see my notes) we find Z ...

$$Z = \prod_{\nu=-\infty}^{\infty} \prod_{\gamma} \int d\tilde{\phi}^*_{\gamma,\nu}\, d\tilde{\phi}_{\gamma,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}$$

$$S[\tilde{\phi}^*,\tilde{\phi}] = -\sum_{\alpha,\beta,\nu} \tilde{\phi}^*_{\alpha,\nu}\, e^{i\omega_\nu \epsilon}\, G^{-1}_{0,\alpha\beta}(i\omega_\nu)\, \tilde{\phi}_{\beta,\nu} + K_1[\tilde{\phi}^*,\tilde{\phi}]$$

$$\mathbf{G}_0^{-1}(i\omega_\nu) = i\omega_\nu - \frac{\mathbf{t}-\mu}{\hbar}$$

Fourier transform of S

- After some algebra (see my notes) we find Z ...

$$Z = \prod_{\nu=-\infty}^{\infty} \prod_{\gamma} \int d\tilde{\phi}^*_{\gamma,\nu}\, d\tilde{\phi}_{\gamma,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}$$

$$S[\tilde{\phi}^*,\tilde{\phi}] = -\sum_{\alpha,\beta,\nu} \tilde{\phi}^*_{\alpha,\nu}\, e^{i\omega_\nu \epsilon}\, G^{-1}_{0,\alpha\beta}(i\omega_\nu)\, \tilde{\phi}_{\beta,\nu} + K_1[\tilde{\phi}^*,\tilde{\phi}]$$

$$\mathbf{G}_0^{-1}(i\omega_\nu) = i\omega_\nu - \frac{\mathbf{t}-\mu}{\hbar}$$

... and the Green's function

$$G_{\alpha,\beta}(i\omega_\nu) = -\frac{\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\nu}\, d\tilde{\phi}_{\gamma,\nu}\, \tilde{\phi}_{\alpha,\nu}\, \tilde{\phi}^*{}_{\beta,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}{\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\nu}\, d\tilde{\phi}_{\gamma,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}},$$

Change of perspective

The Green's function can be represented as a Grassmann functional integral

$$G_{\alpha,\beta}(i\omega_\nu) = -\frac{\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, \tilde{\phi}_{\alpha,\nu}\, \tilde{\phi}^*_{\beta,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}{\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}},$$

$$S[\tilde{\phi}^*,\tilde{\phi}] = -\sum_{\alpha,\beta,\nu} \tilde{\phi}^*_{\alpha,\nu}\, e^{i\omega_\nu \epsilon}\, G^{-1}_{0,\alpha\beta}(i\omega_\nu)\, \tilde{\phi}_{\beta,\nu} + K_1[\tilde{\phi}^*,\tilde{\phi}]$$

- But $\mathbf{G}_0$, $\mathbf{G}$, Σ are 'sets of complex matrices': $F_{\alpha,\beta}(i\omega_\nu)$, $F \in \{G_0, G, \Sigma\}$

  - now take the above as definition of a functional $\mathcal{G}[\mathbf{G}_0^{-1}]$

This functional has K_1 - the interaction part of H - as an implicit parameter

We will now introduce a number of functionals

All of these have K_1 as an implicit parameter

None of them depends on K_0

More functionals

$$Z = \prod_{\nu=-\infty}^{\infty} \prod_{\gamma} \int d\tilde{\phi}^*_{\gamma,\nu}\, d\tilde{\phi}_{\gamma,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})},$$

$$S[\tilde{\phi}^*,\tilde{\phi}] = -\sum_{\gamma,\nu} \tilde{\phi}^*_{\alpha,\nu}\, e^{i\omega_\nu \epsilon}\, G^{-1}_{0,\alpha\beta}(i\omega_\nu)\, \tilde{\phi}_{\beta,\nu} + K_1[\tilde{\phi}^*,\tilde{\phi}]$$

Another functional

$$\Omega[\mathbf{G}_0^{-1}] = -\frac{1}{\beta} \ln\left(\prod_{\nu=-\infty}^{\infty} \prod_{\gamma} \int d\tilde{\phi}^*_{\gamma,\nu}\, d\tilde{\phi}_{\gamma,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})} \right)$$

Let $\mathbf{G}_0^{-1}(i\omega_\nu) = i\omega_\nu - \frac{\mathbf{t}-\mu}{\hbar}$ (physical noninteracting Green's function)

$\Rightarrow \Omega[\mathbf{G}_0^{-1}]$ is the grand canonical potential for $K = K_0 + K_1$

Functional derivative of Ω

$$\Omega[\mathbf{G}_0^{-1}] = -\frac{1}{\beta} \ln\left(\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})} \right)$$

$$S[\tilde{\phi}^*,\tilde{\phi}] = -\sum_{\alpha,\beta,\nu} \tilde{\phi}^*_{\alpha,\nu}\, e^{i\omega_\nu \epsilon}\, G^{-1}_{0,\alpha\beta}(i\omega_\nu)\, \tilde{\phi}_{\beta,\nu} + K_1[\tilde{\phi}^*,\tilde{\phi}]$$

$$\Rightarrow \frac{\partial S[\tilde{\phi}^*,\tilde{\phi}]}{\partial G^{-1}_{0,\alpha\beta}(i\omega_\nu)} = -e^{i\omega_\nu\epsilon}\, \tilde{\phi}^*_{\alpha,\nu}\, \tilde{\phi}_{\beta,\nu} = e^{i\omega_\nu\epsilon}\, \tilde{\phi}_{\beta,\nu}\, \tilde{\phi}^*_{\alpha,\nu}$$

$$\Rightarrow \frac{\partial \Omega[\mathbf{G}_0^{-1}]}{\partial G^{-1}_{0,\alpha,\beta}(i\omega_\nu)} = \frac{e^{i\omega_\nu\epsilon}}{\beta} \frac{\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, \tilde{\phi}_{\beta,\nu}\, \tilde{\phi}^*_{\alpha,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}{\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}},$$

$$= -\frac{1}{\beta}\, e^{i\omega_\nu\epsilon}\, \mathcal{G}[\mathbf{G}_0^{-1}]_{\beta,\alpha}(i\omega_\nu)$$

One last functional ...

$$\mathcal{G}[\mathbf{G}_0^{-1}] = -\frac{\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, \tilde{\phi}_{\alpha,\nu}\, \tilde{\phi}^*_{\beta,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}{\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}},$$

$$S[\tilde{\phi}^*,\tilde{\phi}] = -\sum_{\gamma,\nu} \tilde{\phi}^*_{\alpha,\nu}\, e^{i\omega_\nu \epsilon}\, G^{-1}_{0,\alpha\beta}(i\omega_\nu)\, \tilde{\phi}_{\beta,\nu} + K_1[\tilde{\phi}^*,\tilde{\phi}]$$

- Let $\Sigma_{\alpha,\beta}(i\omega_\nu)$ be a 'self-energy'
- Let $\mathbf{G}[\Sigma]$ be the solution of the equation $\mathcal{G}[\mathbf{G}^{-1}[\Sigma] + \Sigma] = \mathbf{G}[\Sigma]$
- For a true Green's function $\mathbf{G}$ and self-energy Σ : $\mathbf{G}^{-1} = \mathbf{G}_0^{-1} - \Sigma$

$$\mathcal{G}[\mathbf{G}^{-1} + \Sigma] = \mathcal{G}[\mathbf{G}_0^{-1}] = \mathbf{G} \quad \rightarrow \quad \mathbf{G}[\Sigma] = \mathbf{G}$$

The Luttinger-Ward functional

$$\mathcal{G}[\mathbf{G}_0^{-1}] = -\frac{\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, \tilde{\phi}_{\alpha,\nu}\, \tilde{\phi}^*_{\beta,\nu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}{\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})}} \to \mathbf{G}$$

$$\Omega[\mathbf{G}_0^{-1}] = -\frac{1}{\beta} \ln \left(\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu}\, d\tilde{\phi}_{\gamma,\mu}\, e^{-S(\tilde{\phi}^*,\tilde{\phi})} \right) \to \Omega$$

$$\mathcal{G}[\mathbf{G}^{-1}[\Sigma] + \Sigma] = \mathbf{G}[\Sigma] \to \mathbf{G}$$

The Luttinger-Ward functional is

$$F[\Sigma] = \Omega\left[\, \mathbf{G}[\Sigma]^{-1} + \Sigma \,\right] + \frac{1}{\beta} \sum_\lambda e^{i\omega_\lambda \epsilon} \ln \det \mathbf{G}[\Sigma]^{-1}(i\omega_\lambda)$$

$$\to \Omega + \frac{1}{\beta} \sum_\lambda e^{i\omega_\lambda \epsilon} \ln \det \mathbf{G}^{-1}(i\omega_\lambda)$$

- (using $\mathbf{G}[\Sigma]^{-1} + \Sigma \to \mathbf{G}_0$)

The Luttinger-Ward functional was

$$F[\Sigma] = \Omega\Big[\underbrace{\mathbf{G}[\Sigma]^{-1}+\Sigma}_{\mathbf{G}_0}\Big] + \frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon} \ln \det \mathbf{G}[\Sigma]^{-1}(i\omega_\lambda)$$

We want to calculate $\dfrac{\partial F[\Sigma]}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)}$

For a function of a matrix $\mathbf{M}(x)$ the chain rule gives

$$\frac{\partial f(\mathbf{M})}{\partial x} = \sum_{\gamma,\delta} \frac{\partial f}{\partial M_{\gamma,\delta}} \frac{\partial M_{\gamma,\delta}}{\partial x}$$

$$\Rightarrow \frac{\partial \Omega}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} = \sum_{\gamma,\delta,\lambda} \frac{\partial \Omega}{\partial \mathbf{G}_{0,\gamma,\delta}(i\omega_\lambda)} \left[\frac{\partial G^{-1}_{\gamma,\delta}(i\omega_\lambda)}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} + \frac{\partial \Sigma_{\gamma,\delta}(i\omega_\lambda)}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)}\right]$$

Functional derivative of Ω

$$\Omega[\mathbf{G}_0^{-1}] = -\frac{1}{\beta} \ln \left(\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu} \, d\tilde{\phi}_{\gamma,\mu} \, e^{-S(\tilde{\phi}^*,\tilde{\phi})} \right)$$

$$S[\tilde{\phi}^*,\tilde{\phi}] = -\sum_{\alpha,\beta,\nu} \tilde{\phi}^*_{\alpha,\nu} \, e^{i\omega_\nu \epsilon} \, G^{-1}_{0,\alpha\beta}(i\omega_\nu) \, \tilde{\phi}_{\beta,\nu} + K_1[\tilde{\phi}^*,\tilde{\phi}]$$

$$\Rightarrow \frac{\partial S[\tilde{\phi}^*,\tilde{\phi}]}{\partial G^{-1}_{0,\alpha\beta}(i\omega_\nu)} = -e^{i\omega_\nu \epsilon} \, \tilde{\phi}^*_{\alpha,\nu} \, \tilde{\phi}_{\beta,\nu} = e^{i\omega_\nu \epsilon} \, \tilde{\phi}_{\beta,\nu} \, \tilde{\phi}^*_{\alpha,\nu}$$

$$\Rightarrow \frac{\partial \Omega[\mathbf{G}_0^{-1}]}{\partial G^{-1}_{0,\alpha,\beta}(i\omega_\nu)} = \frac{e^{i\omega_\nu \epsilon}}{\beta} \frac{\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu} \, d\tilde{\phi}_{\gamma,\mu} \, \tilde{\phi}_{\beta,\nu} \, \tilde{\phi}^*_{\alpha,\nu} \, e^{-S(\tilde{\phi}^*,\tilde{\phi})}}{\prod_\mu \prod_\gamma \int d\tilde{\phi}^*_{\gamma,\mu} \, d\tilde{\phi}_{\gamma,\mu} \, e^{-S(\tilde{\phi}^*,\tilde{\phi})}},$$

$$= -\frac{1}{\beta} \, e^{i\omega_\nu \epsilon} \, \mathcal{G}[\mathbf{G}_0^{-1}]_{\beta,\alpha}(i\omega_\nu)$$

We found

$$\frac{\partial \Omega}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} = \sum_{\gamma,\delta,\lambda} \frac{\partial \Omega}{\partial \mathbf{G}_{0,\gamma,\delta}(i\omega_\lambda)} \left[\frac{\partial G^{-1}_{\gamma,\delta}(i\omega_\lambda)}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} + \frac{\partial \Sigma_{\gamma,\delta}(i\omega_\lambda)}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} \right]$$

$$= -\frac{1}{\beta} \sum_{\gamma,\delta,\lambda} e^{i\omega_\lambda \epsilon} \mathcal{G}\left[\mathbf{G}_o\right]_{\delta,\gamma}(i\omega_\lambda) \left[\frac{\partial G^{-1}_{\gamma,\delta}(i\omega_\lambda)}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} + \delta_{\gamma,\alpha}\,\delta_{\delta,\beta}\,\delta_{\lambda,\nu} \right]$$

$$= -\frac{1}{\beta} \sum_{\gamma,\delta,\lambda} e^{i\omega_\lambda \epsilon} \mathcal{G}\left[\mathbf{G}_o\right]_{\delta,\gamma}(i\omega_\lambda) \frac{\partial G^{-1}_{\gamma,\delta}(i\omega_\lambda)}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)}$$

$$-\frac{1}{\beta}\, e^{i\omega_\nu \epsilon} \mathcal{G}\left[\mathbf{G}_o\right]_{\beta,\alpha}(i\omega_\nu)$$

$$F[\Sigma] \quad = \quad \Omega \left[\mathbf{G}[\Sigma]^{-1} + \Sigma \right] + \frac{1}{\beta} \sum_{\lambda} e^{i\omega_\lambda \epsilon} \ln \det \mathbf{G}[\Sigma]^{-1}(i\omega_\lambda)$$

We use the identity (see Appendix of my notes) ...

$$\frac{\partial \ln(\det \mathbf{A})}{\partial A_{\alpha,\beta}} = A^{-1}_{\beta,\alpha}$$

... and again the chain rule (replacing $\mathbf{A} \rightarrow \mathbf{M}^{-1}$)

$$\frac{\partial \ln \det \mathbf{M}^{-1}}{\partial x} = \sum_{\gamma,\delta} \frac{\partial \ln \det \mathbf{M}^{-1}}{\partial M^{-1}_{\gamma,\delta}} \frac{\partial M^{-1}_{\gamma,\delta}}{\partial x} = \sum_{\gamma,\delta} M_{\delta,\gamma} \frac{\partial M^{-1}_{\gamma,\delta}}{\partial x}$$

and find

$$\frac{\partial \ln \det \mathbf{G}[\Sigma]^{-1}(i\omega_\lambda)}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} = \sum_{\gamma,\delta,\lambda} G[\Sigma]_{\delta,\gamma}(i\omega_\lambda) \frac{\partial G^{-1}[\Sigma]_{\gamma,\delta}(i\omega_\lambda)}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)}$$

$$F[\Sigma] = \Omega\left[\underbrace{\mathbf{G}[\Sigma]^{-1} + \Sigma}_{\mathbf{G}_0}\right] + \frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon} \ln \det \mathbf{G}[\Sigma]^{-1}(i\omega_\lambda)$$

$$\frac{\partial F[\Sigma]}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} = -\frac{1}{\beta}\sum_{\gamma,\delta,\lambda} e^{i\omega_\lambda \epsilon} \mathcal{G}\left[\mathbf{G}_o\right]_{\delta,\gamma}(i\omega_\lambda) \frac{\partial G[\Sigma]^{-1}_{\gamma,\delta}(i\omega_\lambda)}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)}$$

$$-\frac{1}{\beta} e^{i\omega_\nu \epsilon} \mathcal{G}\left[\mathbf{G}_o\right]_{\beta,\alpha}(i\omega_\nu)$$

$$+\frac{1}{\beta}\sum_{\gamma,\delta,\lambda} e^{i\omega_\lambda \epsilon} G[\Sigma]_{\delta,\gamma}(i\omega_\lambda) \frac{\partial G[\Sigma]^{-1}_{\gamma,\delta}(i\omega_\lambda)}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)}$$

$$\rightarrow \quad -\frac{1}{\beta} e^{i\omega_\nu \epsilon} G_{\beta,\alpha}(i\omega_\nu)$$

What we found so far

- There exists a functional $F[\Sigma]$ of the self energy with the properties

$$\Omega = -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon} \ \mathrm{ln\,det}\left(\mathbf{G}^{-1}(i\omega_\lambda)\right) + F[\Sigma]$$

$$\frac{\partial F[\Sigma]}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} = -\frac{1}{\beta}\, e^{i\omega_\nu \epsilon} G_{\beta,\alpha}(i\omega_\nu)$$

- $F[\Sigma]$ has the interaction part K_1 as an implicit parameter
- $F[\Sigma]$ does not depend on the noninteracting part K_0 in the Hamiltonian

Stationarity property

$$\Omega \quad = \quad -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon} \ \ln\det\left(\mathbf{G}_0^{-1}(i\omega_\lambda) - \Sigma(i\omega_\lambda)\right) + F[\Sigma]$$

We want to calculate $\dfrac{\partial\Omega}{\partial\Sigma_{\alpha,\beta}(i\omega_\nu)}$

We have shown

$$\frac{\partial F[\Sigma]}{\partial\Sigma_{\alpha,\beta}(i\omega_\nu)} \quad = \quad -\frac{1}{\beta}\, e^{i\omega_\nu\epsilon}\, G_{\beta,\alpha}(i\omega_\nu)$$

We use $\mathbf{G}^{-1}(i\omega_\nu) = \mathbf{G}_0^{-1}(i\omega_\nu) - \Sigma(i\omega_\nu)$ and

$$\frac{\partial \ln(\det A)}{\partial A_{\alpha,\beta}} = A^{-1}_{\beta,\alpha} \quad \Rightarrow \quad \frac{\partial \ln \ \det \mathbf{G}^{-1}(i\omega_\lambda)}{\partial\Sigma_{\alpha,\beta}(i\omega_\nu)} = -G_{\beta,\alpha}(i\omega_\nu)\ \delta_{\lambda,\nu}$$

Stationarity property

We had

$$\Omega[\Sigma] \;=\; -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\ \ln\det\left(\mathbf{G}^{-1}(i\omega_\lambda)\right) + F[\Sigma].$$

We found

$$\frac{\partial \ln\ \det \mathbf{G}^{-1}(i\omega_\lambda)}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} \;=\; -G_{\beta,\alpha}(i\omega_\nu)\ \delta_{\lambda,\nu}$$

$$\frac{\partial F[\Sigma]}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} \;=\; -\frac{1}{\beta}\ e^{i\omega_\nu \epsilon}\ G_{\beta,\alpha}(i\omega_\nu)$$

Therefore

$$\frac{\partial \Omega}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} \;=\; \frac{1}{\beta}\ e^{i\omega_\nu \epsilon}\ G_{\beta,\alpha}(i\omega_\nu) - \frac{1}{\beta}\ e^{i\omega_\nu \epsilon}\ G_{\beta,\alpha}(i\omega_\nu) = 0$$

Variational principle emerging?

- We have seen that Ω can be expressed as a functional of the self energy ....

$$\Omega[\Sigma] \quad = \quad -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon} \ \ln\det\left(\mathbf{G}_0^{-1}(i\omega_\lambda) - \Sigma(i\omega_\lambda)\right) + F[\Sigma]$$

- ... which is stationary at the exact self-energy

$$\frac{\partial\Omega}{\partial\Sigma_{\alpha,\beta}(i\omega_\nu)} \quad = \quad 0$$

We therefore might choose a 'trial self-energy' of the form ...

$$\Sigma(i\omega_\nu) \quad = \quad const + \int_{-\infty}^{\infty} d\omega \ \frac{\sigma(\omega)}{\omega - i\omega_\nu}.$$

... and derive Euler-Lagrange equation for $\sigma(\omega)$!

Sounds good but we have no explicit expression for $F[\Sigma]$ ...

The Variational Cluster Approximation

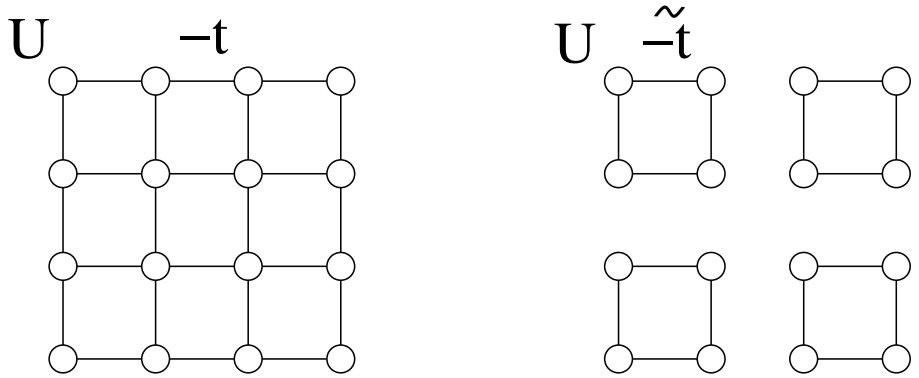
- We recall:
- $F[\Sigma]$ has the interaction part K_1 in the Hamiltonian as implicit parameter
- $F[\Sigma]$ does not depend on the noninteracting part K_0 in the Hamiltonian
- $F[\Sigma]$ is the same for any two systems which have the same interaction part

Variational Cluster Approximation

- Consider the 2D Hubbard model on an infinite square lattice

$$H = -\sum_{i,j} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

- We partition the square lattice into finite clusters - say 2×2



$$\tilde{H} = -\sum_{\{i,j\} \in Cluster} \tilde{t}_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Both systems have the same interaction part $\rightarrow$ they have the same $F[\Sigma]$

- The 2×2 clusters can be solved exactly
- All $|i\rangle$ with $K|i\rangle = K_i|i\rangle$ are known
- We can evaluate the Grand Partition Function $\tilde{Z}$ and $\tilde{\Omega} = -k_B\ T\ log(\tilde{Z})$

$$\tilde{Z} \quad = \quad \sum_i e^{-\beta K_i}$$

- The Green's function $\tilde{G}_{ij}(z)$ $(i,j \in \{1,4\})$ can be calculated
- Inversion gives $\tilde{\mathbf{G}}^{-1}(z)$ and the Dyson equation gives $\tilde{\Sigma}(z)$

$$\tilde{\mathbf{G}}^{-1}(z) \quad = \quad z - \frac{\tilde{\mathbf{t}} - \mu}{\hbar} - \tilde{\Sigma}(z)$$

- Reverting the expression for $\tilde{\Omega}$ gives the numerical value of $F[\tilde{\Sigma}]$

$$F[\tilde{\Sigma}] \quad = \quad \tilde{\Omega} + \lim_{\eta \to 0^+} \frac{1}{\beta} \sum_\nu e^{i\omega_\nu \eta}\ \mathrm{ln}\ \mathrm{det}\left(\tilde{\mathbf{G}}^{-1}(i\omega_\nu\right)$$

- The 2×2 clusters can be solved exactly
- All $|i\rangle$ with $K|i\rangle = K_i|i\rangle$ are known
- We can evaluate the Grand Partition Function $\tilde{Z}$ and $\tilde{\Omega} = -k_B\ T\ log(\tilde{Z})$

$$\tilde{Z} \quad = \quad \sum_i e^{-\beta K_i}$$

- The Green's function $\tilde{G}_{ij}(z)$ $(i,j \in \{1,4\})$ can be calculated
- Inversion gives $\tilde{\mathbf{G}}^{-1}(z)$ and the Dyson equation gives $\tilde{\Sigma}(z)$

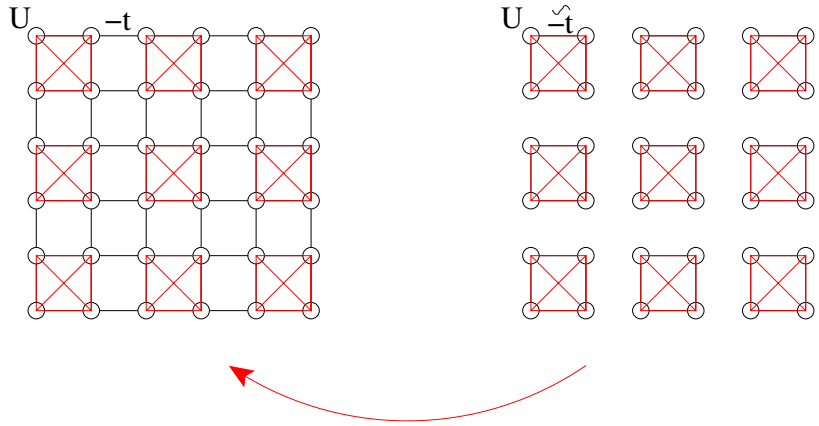
$$\tilde{\mathbf{G}}^{-1}(z) \quad = \quad z - \frac{\tilde{\mathbf{t}} - \mu}{\hbar} - \tilde{\Sigma}(z)$$

- Reverting the expression for $\tilde{\Omega}$ gives the numerical value of $F[\tilde{\Sigma}]$

$$F[\tilde{\Sigma}] \quad = \quad \tilde{\Omega} + \lim_{\eta \to 0^+} \frac{1}{\beta} \sum_\nu e^{i\omega_\nu \eta}\ \mathrm{ln}\ \mathrm{det}\left(\tilde{\mathbf{G}}^{-1}(i\omega_\nu\right)$$

- This gives us the self-energy $\tilde{\Sigma}(\omega)$ and the numerical value of $F[\tilde{\Sigma}]$

- Now we use $\tilde{\Sigma}(z)$ as a 'trial self-energy' for the infinite system



Note: this introduces an artificial supercell structure into the infinite system!

$$\mathbf{G}'_{\mathbf{k}}(z) \quad = \quad \left(z - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar} - \tilde{\Sigma}(z) \right)^{-1}$$

This gives an approximate Grand Canonical Potential for the lattice:

$$\Omega_{latt} \quad = \quad - \lim_{\eta \to 0^+} \frac{1}{\beta} \sum_{\mathbf{k},\nu} e^{i\omega_\nu \eta} \ \ln \ \det \mathbf{G}'_{\mathbf{k}}(i\omega_\nu)^{-1} + N_{Cluster} \ F[\tilde{\Sigma}]$$

Variation of self-energy

$$\mathbf{G}'_{\mathbf{k}}(z) = \left(z - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar} - \tilde{\Sigma}(z) \right)^{-1}$$

$$\Omega_{latt} = - \lim_{\eta \to 0^+} \frac{1}{\beta} \sum_{\mathbf{k},\nu} e^{i\omega_\nu \eta} \ \ln \det \mathbf{G}'_{\mathbf{k}}(i\omega_\nu)^{-1} + N_{Cluster} \, F[\tilde{\Sigma}]$$

The Hamiltonian of the clusters was

$$\tilde{H} = - \sum_{\{i,j\} \in Cluster} \tilde{t}_{ij} \, c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

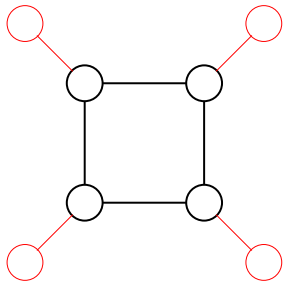
- $\tilde{H}$ must have the same interaction part as the lattice system
- There is nothing that fixes the the single-particle matrix elements $\tilde{t}_{ij}$
- Changing $\tilde{t}_{ij}$ will change $\tilde{\Sigma}(\omega)$ and $F[\tilde{\Sigma}]$ so $\Omega_{latt} = \Omega_{latt}(\tilde{t}_{ij})$
- Then we replace $\dfrac{\delta \Omega_{latt}}{\delta \Sigma} = 0 \quad \rightarrow \quad \dfrac{\partial \Omega_{latt}}{\partial \tilde{t}_{ij}} = 0$

Idea of the Variational Cluster Approximation

- Seek a reference system which has the same K_1 as the original system but consists of finite clusters
- Solve the finite clusters - possible due to small dimension of their Hilbert space
- $\tilde{\Sigma}$ and $F[\tilde{\Sigma}]$ for the reference system can be obtained numerically
- Use $\tilde{\Sigma}$ as a trial self-energy for the original system - possible because we know $F[\tilde{\Sigma}]$
- Variation of $\tilde{\Sigma}$ by varying the parameters of K_0 for the reference system

Bath sites

- We have partitioned the planar model into finite clusters
- We may as well 'decorate' these clusters by 'bath sites'



- A 'bath' site is an orbital ρ without any interaction, i.e. in the interaction term ...

$$K_1 = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} V_{\alpha,\beta,\delta,\gamma} c_\alpha^\dagger \, c_\beta^\dagger \, c_\gamma \, c_\delta$$

...there is no matrix element involving the orbital ρ

- It follows that $\tilde{\Sigma}_{\rho,\alpha} = \tilde{\Sigma}_{\alpha,\rho} = 0$ for any α - $\tilde{\Sigma}$ has no matrix elements involving ρ

Metal-insulator transition in a dimer

For $\mu = \frac{U}{2}$ the Hubbard model has particle-hole symmetry

$$
\begin{aligned}
H - \mu N &= \sum_{i,j,\sigma} t_{ij}\, c^{\dagger}_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_{i=1}^{N} (n_i - 1)(n_i - 1) - N\,\frac{U}{2} \\
n_i &= n_{i,\uparrow} + n_{i,\downarrow}
\end{aligned}
$$

Metal-insulator transition in a dimer

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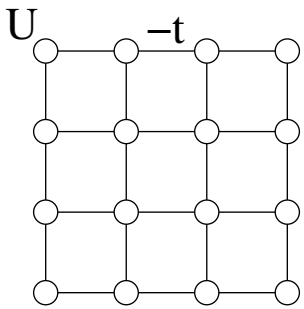
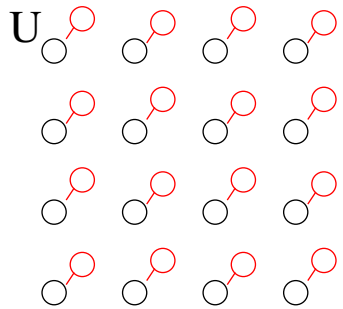
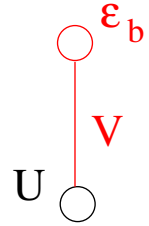
$$\begin{aligned} H - \mu N &= \sum_{i,j,\sigma} t_{ij}\, c^{\dagger}_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_{i=1}^{N} (n_i - 1)(n_i - 1) - N\,\frac{U}{2} \\ n_i &= n_{i,\uparrow} + n_{i,\downarrow} \end{aligned}$$

As reference system we use N dimers - one 'Hubbard site' and one 'bath site'







For $\epsilon_b = \frac{U}{2}$ the Hamiltonian for a dimer also has particle-hole symmetry

$$\tilde{H}_i - \mu N_i = -V \sum_{\sigma} (c^{\dagger}_{i,\sigma} b_{i,\sigma} + b^{\dagger}_{i,\sigma} c_{i,\sigma}) + \frac{U}{2}\,(n_i - 1)(n_i - 1)$$

The Hamiltonian for dimer i is

$$\tilde{H} - \mu N = -V \sum_{\sigma} (c^{\dagger}_{i,\sigma} b_{i,\sigma} + b^{\dagger}_{i,\sigma} c_{i,\sigma}) + \frac{U}{2} (n_i - 1)(n_i - 1)$$

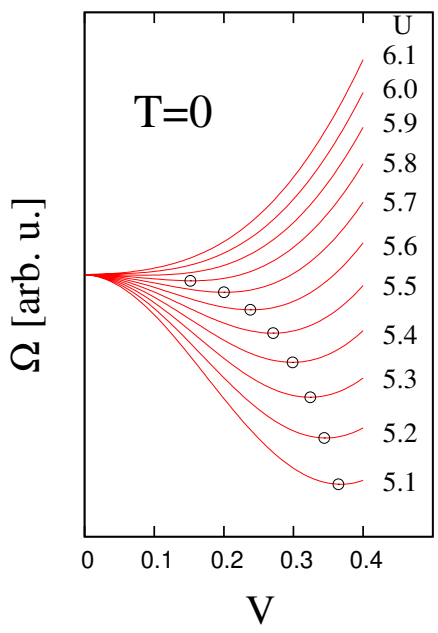
... and the only parameter to be varied is V - now we carry out our programme:

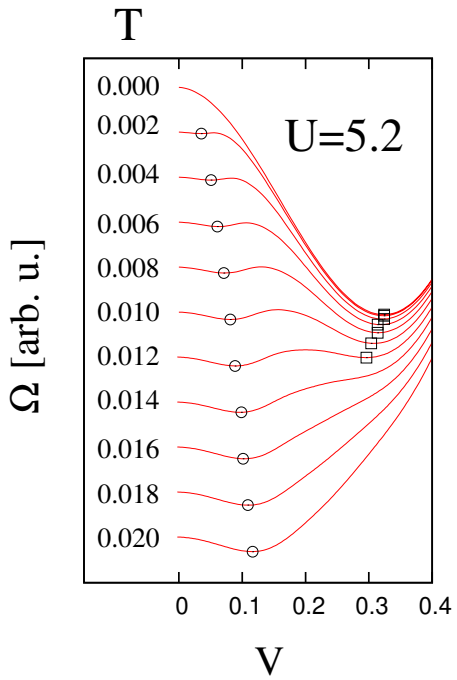
- For each V all eigenstates with $0 \rightarrow 4$ electrons can be calculated
- $\tilde{\Omega}(V)$ and $\tilde{\mathbf{G}}_{i,j}(z, V)$ can be calculated
- $\tilde{\Sigma}(\omega, V)$ is obtained by inverting $\tilde{\mathbf{G}}_{i,j}(z, V)$ and using the Dyson equation
- $F[\tilde{\Sigma}(V)]$ can be obtained from the relation

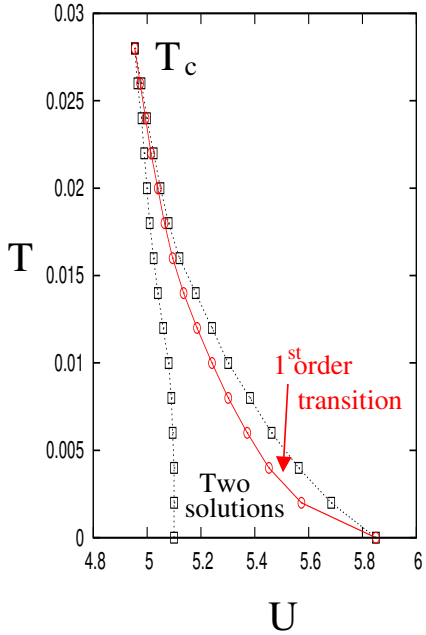
$$F[\tilde{\Sigma}(\omega, V)] = \tilde{\Omega}(V) - \frac{1}{\beta} \sum_{\lambda} e^{i\omega_\lambda \epsilon} \ \ln \det \ \tilde{\mathbf{G}}^{-1}(i\omega_\lambda)$$

- $\tilde{\Sigma}(\omega, V)$ is used a self-energy for the Hubbard-model, $F[\tilde{\Sigma}(\omega, V)]$ is used to calculate $\Omega_{latt}(V)$

The resulting $\Omega_{latt}(V)$ curves and the phase diagram





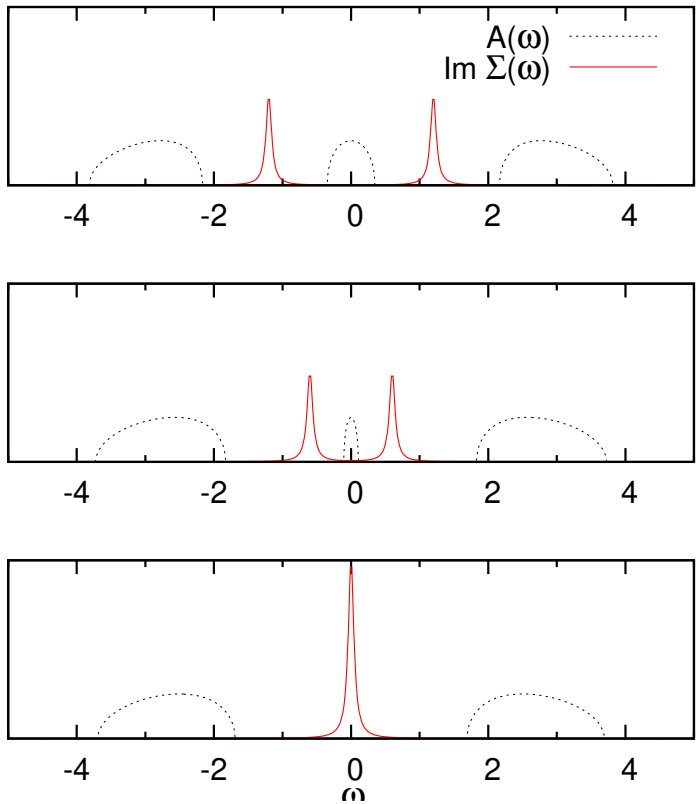


- At $T = 0$: 2^{nd} order phase transition for $U \approx 5.85$ - metal insulator transition
- $U = 5.2$: Coexistence of solutions and 1^{st} order phase transition at $T \approx 0.11$
- Consistent with DMFT, T_c off by a factor of 2

k-integrated spectral function

At $T = 0$ the self-energy of the 'Hubbard orbital' can be evaluated analytically

$$\Sigma(\omega) = \frac{U}{2} + \frac{U^2}{8}\left(\frac{1}{\omega + 3V} + \frac{1}{\omega - 3V}\right)$$



Summary

- 'The' Greens function $\mathbf{G}(z)$ unifies the imaginary time Greens function and the real time Greens function
- The effect of interactions is described by adding the self-energy to $\mathbf{G}_0^{-1}(z)$
- The real time Greens function is the combined photoemission/ inverse photoemission spectrum
- The imaginary time Greens function can be expressed as a Grassmann variable functional integral
- The grand canonical potential of an interacting electron system can be expressed as a functional of its self-energy: $\Omega[\Sigma]$
- $\Omega[\Sigma]$ is stationary at the exact self-energy Σ
- $\Omega[\Sigma]$ involves the Luttinger-Ward functional $F[\Sigma]$ for which no explicit expression is known
- This can be circumvented by introduction of a reference system and combination with numerical methods - Variational Cluster Approximation

Dynamical mean-field theory

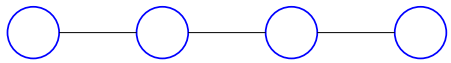
Consider the Hubbard model with N sites and pbc

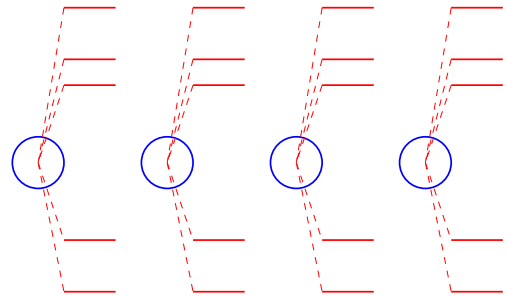
$$H = \sum_{i,j}\sum_{\sigma} t_{i,j}\, c^{\dagger}_{i,\sigma} c_{i,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i\downarrow} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + U \sum_{i} n_{i,\uparrow} n_{i\downarrow}$$

In addition consider the 'reference system'

$$\tilde{H} = \sum_{i=1}^{N} \tilde{H}_i$$

$$\tilde{H}_i = \sum_{\nu} \epsilon_{\nu}\, l^{\dagger}_{i,\nu,\sigma}\, l_{i,\nu,\sigma} + \sum_{\nu} \left(V_{\nu}\, l^{\dagger}_{i,\nu,\sigma} c_{i,\sigma} + H.c. \right) + U\, n_{i,\uparrow} n_{i\downarrow}$$





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In addition consider the 'reference system'

$$\tilde{H} = \sum_{i=1}^{N} \tilde{H}_i$$

$$\tilde{H}_i = \sum_{\nu} \epsilon_{\nu}\, l^{\dagger}_{i,\nu,\sigma}\, l_{i,\nu,\sigma} + \sum_{\nu} \left(V_{\nu}\, l^{\dagger}_{i,\nu,\sigma} c_{i,\sigma} + H.c. \right) + U\, n_{i,\uparrow} n_{i\downarrow}$$

The crucial point: Both models have the same interaction term

$$K_1 = U \sum_{i} n_{i,\uparrow} n_{i\downarrow}$$

Dynamical mean-field theory

- Hubbard model and reference system have the same $F[\Sigma]$
- The 'ligands' $l^{\dagger}_{i,\nu,\sigma}$ are uncorrelated - only $\tilde{\Sigma}_{c,c}(i\omega_\lambda)$ is different from zero

$$\tilde{H}_i = \sum_\nu \epsilon_\nu \, l^{\dagger}_{i,\nu,\sigma} \, l_{i,\nu,\sigma} + \sum_\nu \left(V_\nu \, l^{\dagger}_{i,\nu,\sigma} c_{i,\sigma} + H.c. \right) + U \, n_{i,\uparrow} n_{i\downarrow}$$

- Ω is stationary under variations of the self-energy - we restrict the 'domain of self-energies' to those of the reference system $\tilde{\Sigma}_{c,c}(i\omega_\lambda)$

$$\frac{\partial \Omega}{\partial \Sigma_{\alpha,\beta}(i\omega_\nu)} = 0 \quad \Rightarrow \quad \frac{\partial \Omega}{\partial t} = 0$$

with $t \in \{\epsilon_\nu, V_\nu\}$

Dynamical mean-field theory

Recall: $\tilde{H} = \sum_{i=1}^{N} \tilde{H}_i$

$$\tilde{H}_i = \sum_{\nu} \epsilon_\nu \, l^\dagger_{i,\nu,\sigma} \, l_{i,\nu,\sigma} + \sum_{\nu} \left(V_\nu \, l^\dagger_{i,\nu,\sigma} c_{i,\sigma} + H.c. \right) + U \, n_{i,\uparrow} n_{i\downarrow}$$

We compute the derivative of $F[\tilde{\Sigma}]$ with respect to a parameter $t \in \{\epsilon_\nu, V_\nu\}$

$$\frac{\partial F[\tilde{\Sigma}]}{\partial t} = \sum_{\alpha,\beta} \sum_{\lambda} \frac{\partial F[\tilde{\Sigma}]}{\partial \tilde{\Sigma}_{\alpha,\beta}(i\omega_\lambda)} \frac{\partial \tilde{\Sigma}_{\alpha,\beta}(i\omega_\lambda)}{\partial t}$$

$$= -\frac{1}{\beta} \sum_{\alpha,\beta} \sum_{\lambda} e^{i\omega_\lambda \epsilon} \, \tilde{G}_{\beta,\alpha}(i\omega_\lambda) \frac{\partial \tilde{\Sigma}_{\alpha,\beta}(i\omega_\lambda)}{\partial t}$$

$$= -\frac{2N}{\beta} \sum_{\lambda} e^{i\omega_\lambda \epsilon} \, \tilde{G}_{c,c}(i\omega_\lambda) \frac{\partial \tilde{\Sigma}_{c,c}(i\omega_\lambda)}{\partial t}$$

Dynamical mean-field theory

We apply our general formula ...

$$\Omega[\Sigma] \;=\; -\frac{1}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\ \ln\det\left(\mathbf{G}_0^{-1}(i\omega_\lambda) - \Sigma(i\omega_\lambda)\right) + F[\Sigma].$$

... to the Hubbard model

$$\Omega_{latt} \;=\; -\frac{2}{\beta}\sum_{\mathbf{k}}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\ \ln\left[i\omega_\lambda - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar} - \tilde{\Sigma}_{c,c}(i\omega_\lambda)\right] + 2N\, F[\tilde{\Sigma}]$$

We recall

$$\frac{\partial F[\tilde{\Sigma}]}{\partial t} \;=\; -\frac{2N}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\ \tilde{G}_{c,c}(i\omega_\lambda)\ \frac{\partial \tilde{\Sigma}_{c,c}(i\omega_\lambda)}{\partial t}$$

$$\Rightarrow \frac{\partial \Omega_{latt}}{\partial t} \;=\; \frac{2}{\beta}\sum_{\lambda} e^{i\omega_\lambda \epsilon}\left[\sum_{\mathbf{k}} G(\mathbf{k}, i\omega_\lambda) - N\,\tilde{G}_{c,c}(i\omega_\lambda)\right]\frac{\partial \tilde{\Sigma}_{c,c}(i\omega_\lambda)}{\partial t} = 0$$

Dynamical mean-field theory

We found that for any $t \in \{\epsilon_\nu, V_\nu\}$

$$\frac{\partial \Omega_{latt}}{\partial t} = \frac{2}{\beta} \sum_\lambda e^{i\omega_\lambda \epsilon} \left[\sum_{\mathbf{k}} G(\mathbf{k}, i\omega_\lambda) - N\, \tilde{G}_{c,c}(i\omega_\lambda) \right] \frac{\partial \tilde{\Sigma}_{c,c}(i\omega_\lambda)}{\partial t} = 0$$

The simplest way to solve this is to set for each ω_λ

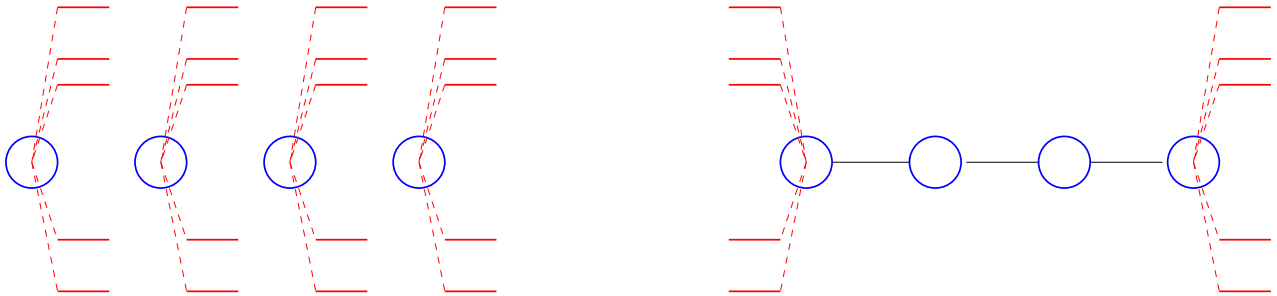
$$\sum_{\mathbf{k}} G(\mathbf{k}, i\omega_\lambda) - N\, \tilde{G}_{c,c}(i\omega_\lambda) = 0$$

$$\Rightarrow \tilde{G}_{c,c}(i\omega_\lambda) = \frac{1}{N} \sum_{\mathbf{k}} G(\mathbf{k}, i\omega_\lambda) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{i\omega_\lambda - \frac{\epsilon_{\mathbf{k}} - \mu}{\hbar} - \tilde{\Sigma}_{c,c}(i\omega_\lambda)}$$

This is precisely the self-consistency equation for Dynamical Mean-Field Theory!

Generalizations

In the same way one can derive cluster generalizations of dynamical mean-field theory



Another way is to numerically evaluate the Luttinger-Ward functional in the reference system - this is the Variational Cluster Approximation

And there is probably more to be discovered...for example even an approximate form of $F[\Sigma]$

Summary

- We have seen that the grand canonical potential of an interacting electron system can be expressed as a functional of its self-energy: $\Omega[\Sigma]$
- This functional is stationary at the exact self-energy
- Unfortunately this involves (the Legendre transform of) the Luttinger-Ward functional for which we do not have any explicit expression
- This problem can be circumvented by combination with numerical methods - a.g. in dynamical mean-field theory or cluster generalizations