# Dual variables: a description of collective phenomena in correlated media

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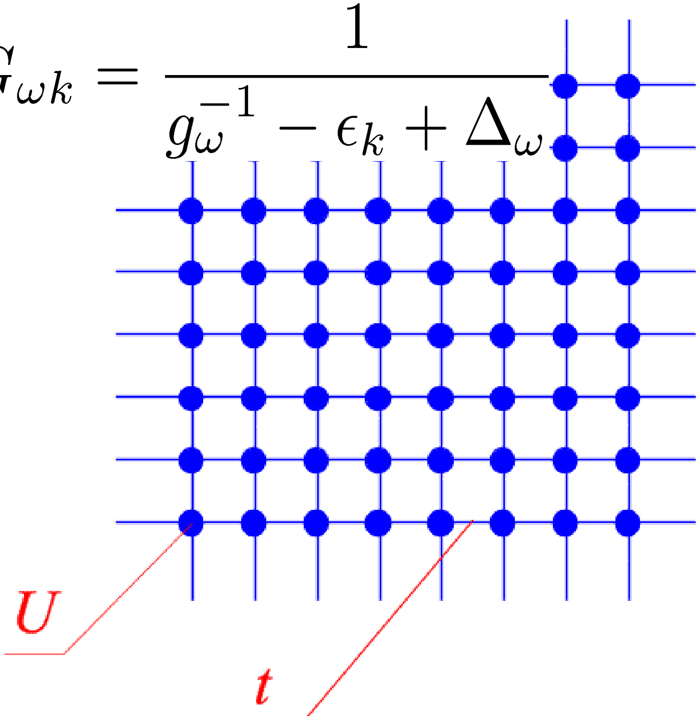
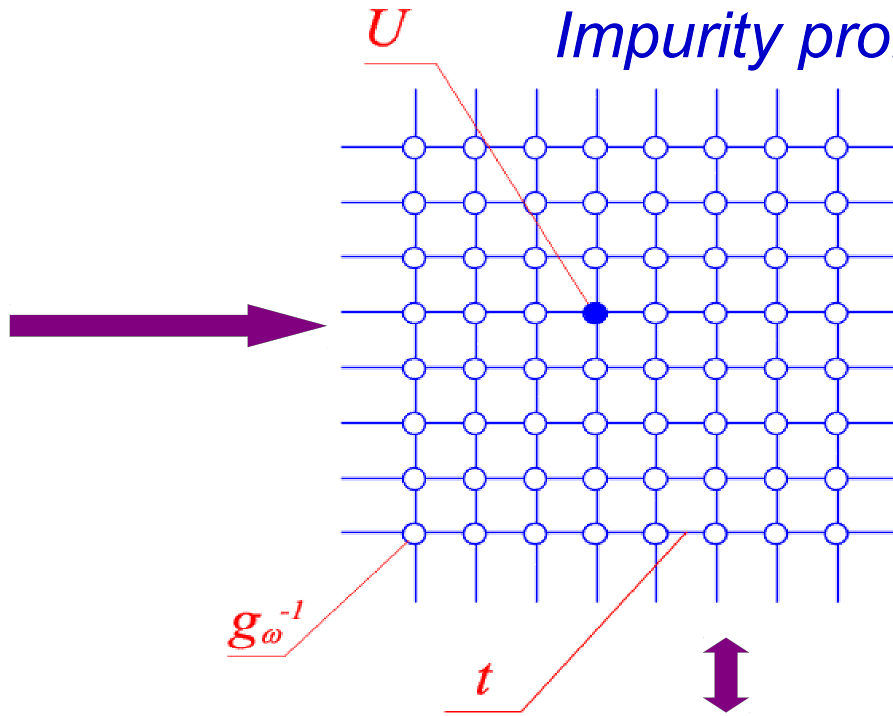
# DMFT

W. Metzner, D. Vollhardt (1989) G. Kotliar, A. Georges (1993)

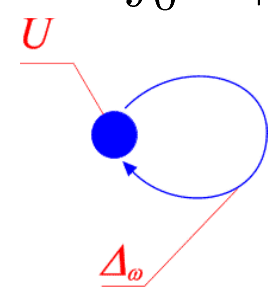
$$G_{\omega k} = \frac{1}{g_\omega^{-1} - \epsilon_k + \Delta_\omega}$$




**Impurity problem:**



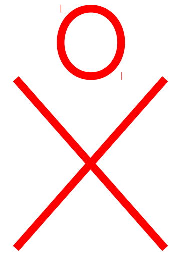

$$S_{imp} = \sum_{\omega,\sigma} (\Delta_\omega - \mu - i\omega) c^*_{\omega,\sigma} c_{\omega,\sigma} + U \int_0^\beta n_{\uparrow\tau} n_{\downarrow\tau} d\tau$$




$$g_\omega = \sum_k \frac{N^{-1}}{g_\omega^{-1} - \epsilon_k + \Delta_\omega}$$

# *EDMFT*

P.Sun, G. Kotliar (2004)



$$S = \sum_r S_{at}[c_r^\dagger, c_r] + \sum_{r,R\neq 0,\omega,\sigma} \varepsilon_R c^\dagger_{r\omega\sigma} c_{r+R\omega\sigma} + \sum_{r,R\neq 0,\Omega} V_{R\Omega} \rho^*_{r\Omega} \rho_{r+R\Omega}$$

$$S_{at} = -\sum_{\omega\sigma} (i\omega + \mu) c^\dagger_{\omega\sigma} c_{\omega\sigma} + U \int_0^\beta c^\dagger_\uparrow c_\uparrow c^\dagger_\downarrow c_\downarrow d\tau$$

$$G_{r\tau} = - < c_{r\tau} c^\dagger_{r=0,\tau=0} >$$

$$X_{r\tau} = - < \rho_{r\tau} \rho^*_{r=0,\tau=0} >$$

Impurity problem

$$S_{imp} = S_{at} + \sum_\omega \Delta_\omega c^\dagger_\omega c_\omega + \sum_\Omega \Lambda_\Omega \rho^*_\Omega \rho_\Omega$$

Self-consistency

$$g_\omega = \sum_k \mathcal{G}_{\omega k},$$

$$\chi_\Omega = \sum_k \mathcal{X}_{\Omega k}$$

EDMFT Green's functions

$$\mathcal{G}_{\omega k} = \frac{1}{g_\omega^{-1} + \Delta_\omega - \epsilon_k}$$

$$\mathcal{X}_{\Omega k} = \frac{1}{\chi_\Omega^{-1} + \Lambda_\Omega - V_k}$$

# Difficulties of EDMFT

Local polarization operator

$$\chi_\Omega = \sum_k \mathcal{X}_{\Omega k} \qquad \mathcal{X}_{\Omega k} = \frac{1}{\chi_\Omega^{-1} + \Lambda_\Omega - V_k}$$

Does not work for collective modes

$$X_{\Omega K} = \frac{1}{(X^0_{\Omega K})^{-1} - V_K}$$

Charge conservation:

$$X^0_{\Omega K} \equiv < nn >_{\Omega K} = \frac{K^2}{\Omega^2} < jj >_{\Omega K}$$

# *Random phase approximation*

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$$X_{K\Omega} = \frac{1}{(X^0_{K\Omega})^{-1} - V_K}$$

Is conservative...

$$X^0_{RPA}(K=0) = -\sum_{\omega k} \frac{1}{i\omega - \epsilon_k} \frac{1}{i(\omega-\Omega) - \epsilon_k} = -\left( \sum_{\omega k} \frac{1}{i\omega - \epsilon_k} - \frac{1}{i(\omega-\Omega) - \epsilon_k} \right) \frac{1}{i\Omega}$$

but only for uncorrelated electrons:

$$-\left( \sum_{\omega k} \frac{1}{i\omega - \epsilon_k - \Sigma_\omega} - \frac{1}{i(\omega-\Omega) - \epsilon_k - \Sigma_{\omega-\Omega}} \right) \frac{1}{i\Omega + \Sigma_{\omega-\Omega} - \Sigma_\omega}$$

# Difficulties of EDMFT - II:

## *Superexchange in Hubbard model*

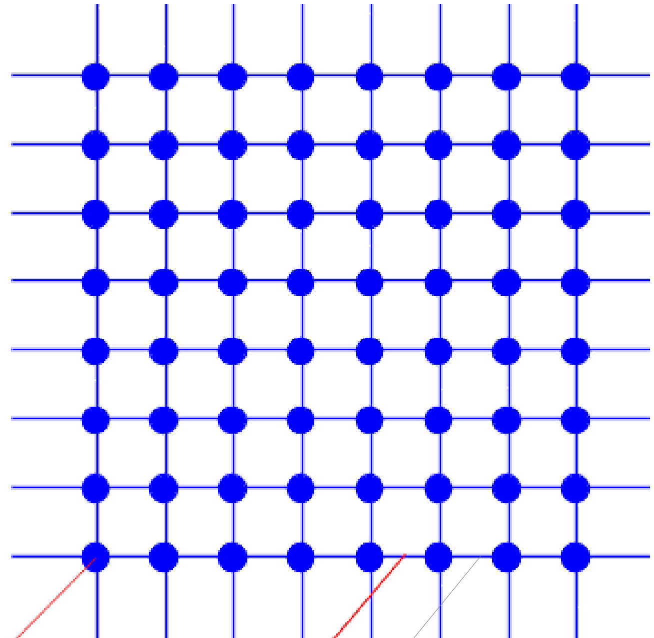
Magnon dispersion

$$\chi_\Omega = \sum_k \frac{1}{\chi_\Omega^{-1} + \Lambda_\Omega - J_k}$$

$\chi = <s\ s>$

$$S_{imp} = S_{at} + \sum_\omega \Delta_\omega c^\dagger_\omega c_\omega + \sum_\Omega \Lambda_\Omega \rho^*_\Omega \rho_\Omega$$

0



$U$

$t$

$J_{ij} = \frac{t^2}{U}$

$V$=0 EDMFT Λ=0

In EDMFT, superexchange should be introduced ad hoc

# *From bosonic field to bosonic modes*

Desired theory:

$$\chi_\Omega = \sum_k \mathcal{X}_{\Omega k} \qquad X_{\Omega K} = \frac{1}{\chi_\Omega^{-1} + \Lambda_\Omega - V_K - \Pi'_{\Omega K}}$$

$$S_{imp} = S_{at} + \sum_\omega \Delta_\omega c_\omega^\dagger c_\omega + \sum_\Omega \Lambda_\Omega \rho_\Omega^* \rho_\Omega$$

$\Lambda$ without V

$V$=0 ⟺ EDMFT ⟺ $\Lambda$=0

# Dual bosons

$$S=\sum_r S_{imp}[c_r^\dagger,c_r]+\sum_{\omega,k,\sigma}(\varepsilon_k-\Delta_{\omega\sigma})\,c_{\omega k\sigma}^\dagger c_{\omega k\sigma}+\sum_{\Omega,k,j,j'}\left(V_{\Omega k}^{jj'}-\Lambda_\Omega^{jj'}\right)\rho_{\Omega kj}^*\rho_{\Omega kj'}$$

$$\int D\left[c^\dagger,c\right]e^{c^\dagger Ec}=\int D\left[c^\dagger,c\right]\det\left(\alpha_f^{-1}E\alpha_f^{-1}\right)\int D\left[f^\dagger,f\right]e^{\{-f^\dagger\alpha_f E^{-1}\alpha_f f+f^\dagger\alpha_f c+c^\dagger\alpha_f f\}}$$

$$\int D\left[\rho^*,\rho\right]e^{\rho^*W\rho}=\int D\left[\rho^*,\rho\right]\det\left(\alpha_b W^{-1}\alpha_b\right)\int D\left[\eta^*,\eta\right]e^{\{-\eta^*\alpha_b W^{-1}\alpha_b\eta+\eta^*\alpha_b\rho+\rho^*\alpha_b\eta\}},$$

$$S=-\sum_{\omega k}\tilde{\mathcal{G}}_{\omega k}^{-1}f_{\omega k}^\dagger f_{\omega k}-\sum_{\Omega k}\tilde{\mathcal{X}}_{\Omega k}^{-1}\eta_{\Omega k}^*\eta_{\Omega k}+\sum_i\tilde{U}[\eta_i,f_i,f_i^\dagger]$$

$$\tilde{\mathcal{G}}_{\omega k}^{-1}=g_\omega^{-1}(\varepsilon_k-\Delta_\omega)^{-1}g_\omega^{-1}-g_\omega^{-1}$$

$$\tilde{\mathcal{X}}_{\Omega k}^{-1}=\chi_\Omega^{-1}(V_k-\Lambda_\Omega)^{-1}\chi_\Omega^{-1}-\chi_\Omega^{-1}$$

$$\tilde{U}[\eta,f,f^\dagger]=\sum_{\omega\Omega}\left(\lambda_{\omega\Omega}\eta_\Omega^*f_{\omega+\Omega}^\dagger f_\omega+\lambda_{\omega\Omega}^*\eta_\Omega f_\omega^\dagger\ f_{\omega+\Omega}\right)+\frac{1}{4}\sum_{\omega\omega'\Omega}\gamma_{\omega\omega'\Omega}f_{\omega+\Omega}^\dagger f_{\omega'-\Omega}^\dagger f_\omega f_{\omega'}+\ldots$$

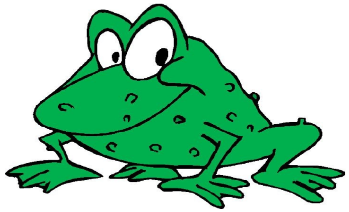
$$\gamma_{\omega\omega'\Omega}=\frac{<c_{\omega+\Omega}c_{\omega'-\Omega}c_\omega^\dagger c_{\omega'}^\dagger>_{imp}-g_\omega g_{\omega'}(\delta_{\Omega+\omega-\omega'}-\delta_\Omega)}{g_{\omega+\Omega}g_{\omega'-\Omega}g_\omega g_{\omega'}}\qquad\lambda_{\omega\Omega}=\frac{-<c_{\omega+\Omega}c_\omega^\dagger\rho_\Omega>_{imp}-<\rho>_{imp}\,g_\omega\delta_\Omega}{g_\omega g_{\omega+\Omega}\chi_\Omega}$$

# *Interpretation*

Hamiltonian action with local in time, but large (tall and beatiful) U

(troubles,troubles)

Non-Hamiltonian action with retarded V, formally including all ordres of interaction (but negligible!)



(can be hidden in your pocket, not much food required)

# Conservative theory

Conservation laws are related with gauge invariance:

$$c_{r\tau} \to c_{r\tau} e^{i\Lambda_{r\tau}}$$

DMFT is conservative, if the susceptibility is calculated self-consistently,

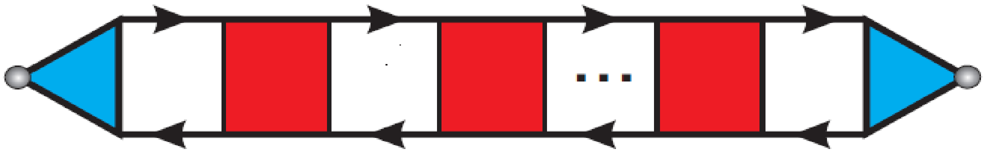
$\delta\epsilon_{\omega k} \to \delta\Delta_{\omega}, \delta g_{\omega}$ preserving $g_{\omega} = \sum_k G_{\omega k}$

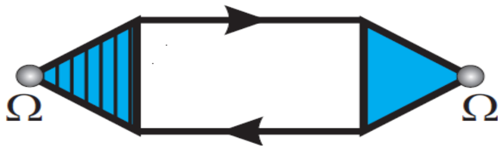
It gives (indices ω, ω' are omitted!):

$$\frac{1}{X_{\Omega K}} - \frac{1}{x_{\Omega}} = \frac{1}{X^{0}_{\Omega K}} - \frac{1}{x^{0}_{\Omega}}$$

$$X^{0,\omega}_{\Omega K} = -\sum_k \mathcal{G}_{\omega k}\mathcal{G}_{\omega+\Omega k+K}$$
$$x^{0,\omega}_{\Omega K} = -g_{\omega} g_{\omega+\Omega}.$$

Thus calculated susceptibility should be used instead of RPA empty loop.
In dual variables, it corresponds to the ladder summation

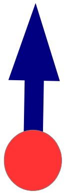




# Local moment

*a case of large impurity vertex*

Isolated atom



$$g_{at} = \frac{-i\omega}{\omega^2 + (U/2)^2}$$

$$\gamma = \beta U^2 \delta_{\Omega 0}$$

Slow dynamics of the local moment is not reflected in the Green's function, but do contribute vertex part

Strong coupling limit

$$\gamma = \gamma_\Omega$$

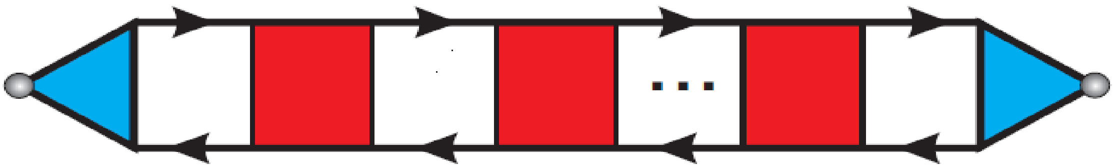
$$\chi_\Omega = \chi_\Omega^{(0)} \gamma_\Omega \chi_\Omega^{(0)}$$

$$\lambda_\Omega = (\chi_\Omega^{(0)})^{-1}$$

$$\chi_\Omega^{(0)} \equiv -\sum_{\omega\sigma} g_\omega g_{\Omega+\omega}$$

# *Ladder summation*

## *strong-coupling limit*



$$\chi_\Omega = \chi_\Omega^{(0)} \gamma_\Omega \chi_\Omega^{(0)}$$

$$\lambda_\Omega = (\chi_\Omega^{(0)})^{-1}$$

$$\Pi'_{\Omega K} = \left[ \left( \lambda \frac{\tilde{X}^{(0)}_{\Omega K}}{1 - \gamma_\Omega \tilde{X}^{(0)}_{\Omega K}} \lambda \right)^{-1} + \chi_\Omega \right]^{-1}$$

$$\Pi'_{\Omega K} = \lambda_\Omega \tilde{X}^0_{\Omega K} \lambda_\Omega$$

$\gamma_\Omega$ drops out!

**RPA would put $J_k$ in a denominator!**

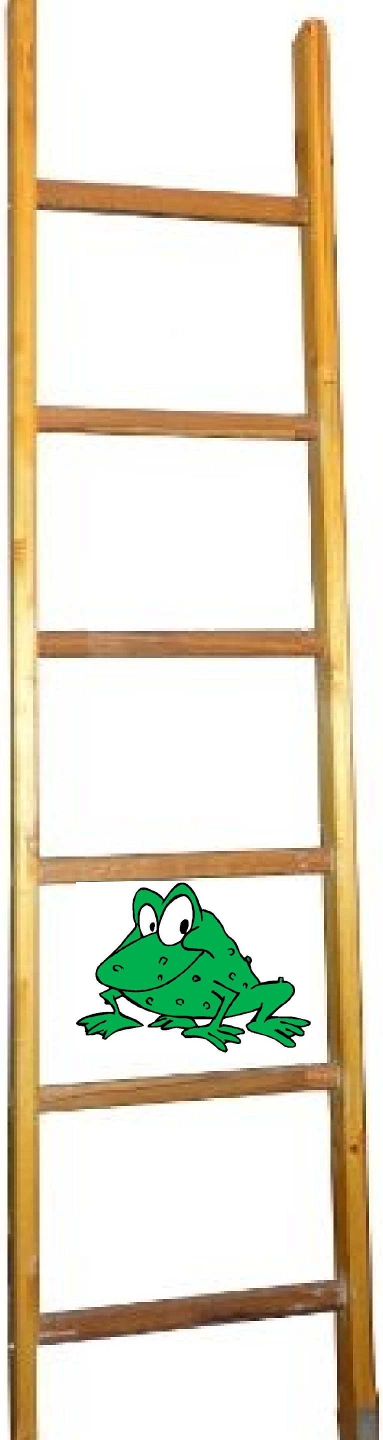
$$\frac{1}{\chi_\Omega^{-1} + \Lambda_\Omega - J_k}$$

$$g = g_{at}$$

$$\tilde{X}_{\Omega=0} = \frac{t^2}{4U^3}$$

$$\chi^{(0)}_{\Omega=0} = \frac{1}{2U}$$

$J_{ij} = \frac{t^2}{U}$ for nearest neighbors



# Conclusions

For DMFT-based theories with bosons,
dual ladder summation
is a “minimal” conserving theory,
similar to RPA for free electrons

The theory includes slow dynamics of local momenta (e.g. superexchange)