Functional RG within Keldysh formalism

Severin G. Jakobs, Mikhail Pletyukhov, Herbert Schoeller

RNTHAACHEN JARA



Matsubara and Keldysh formalism

Restrictions of Matsubara formalism

- analytic continuation to real frequencies required
- does not allow for nonequilibrium





Keldysh formalism



 \rightarrow particle distribution:

$$g^{\mathsf{K}} = 2\pi i \left[2f(\omega) - 1 \right] \delta(\omega - \epsilon)$$

n-particle Green Functions



Causality



Causality

• $G^{1...1|1...1} \equiv 0$

•
$$G^{21...1|1...1}(\omega_2 \dots \omega_n | \omega')$$
 analytic in

$$\begin{cases} \text{lhp of } \omega_2 \dots \omega_n \\ \text{uhp of } \omega'_1 \dots \omega'_n \end{cases}$$

• 2n fully retarded GFs:

 $G^{21...1|1...1}, \ldots, G^{1...1|1...12}$

For vertex functions exchange $1 \leftrightarrow 2$. • $\gamma^{2...2|2...2} \equiv 0$ • $\gamma^{12...2|2...2}(\omega'_2 \dots \omega'_n | \omega)$ analytic in $\begin{cases} \text{lhp of } \omega'_2 \dots \omega'_n \\ \text{uhp of } \omega_1 \dots \omega_n \end{cases}$ • 2n fully retarded VFs:

 $\gamma^{12...2|2...2}, \ldots, \gamma^{2...2|2...21}$

Example: n = 1 $G^{1|1} \equiv 0$ $G^{\text{Ret}}(\omega') = G^{2|1}(t=0|\omega')$ analytic in uhp of ω' $G^{\text{Av}}(\omega) = G^{1|2}(\omega|t'=0)$ analytic in lhp of ω $\Sigma^{2|2} \equiv 0$ $\Sigma^{\text{Ret}}(\omega) = \Sigma^{1|2}(t'=0|\omega)$ analytic in uhp of ω $\Sigma^{\text{Av}}(\omega') = \Sigma^{2|1}(\omega'|t=0)$ analytic in lhp of ω'

Kubo Martin Schwinger conditions

[For real bosons: Chou et. al., Phys. Rep. 118, 1 (1985)]



Kubo Martin Schwinger conditions

[For real bosons: Chou et. al., Phys. Rep. 118, 1 (1985)]



Fluctuation dissipation theorem

$$e^{\beta\Delta^{i|i'}(\omega|\omega')} G^{i|i'}(\omega|\omega') = \zeta^{m^{i|i'}} \widetilde{G}^{\overline{i}|\overline{i'}}(\omega|\omega') \quad \text{with} \quad \Delta^{i|i'}(\omega|\omega') = \sum_{i'_k = +} \omega'_k - \sum_{i_k = +} \omega_k$$

Special case
$$n = 1$$
:
 $\widetilde{G}^{i|i'} = G^{i'|i}$

$$\Rightarrow e^{\beta \Delta^{i|i'}(\omega|\omega')} G^{i|i'}(\omega|\omega') = \zeta^{m^{i|i'}} G^{i'|i}(\omega|\omega'), \quad n = 1$$

$$\Rightarrow G^{<}(\omega) = \zeta e^{-\beta \omega} G^{>}(\omega)$$

$$\Rightarrow G^{\mathsf{K}}(\omega) = [1 + 2\zeta n_{\zeta}(\omega)] [G^{\mathsf{Ret}}(\omega) - G^{\mathsf{Av}}(\omega)]$$

$$\boxed{n_{\zeta}(\omega) = \frac{1}{e^{\beta \omega} - \zeta}}$$

Time reversal

$$e^{\beta\Delta^{i|i'}(\omega|\omega')} G^{i|i'}(\omega|\omega') = \zeta^{m^{i|i'}} \widetilde{G}^{\overline{i}|\overline{i}'}(\omega|\omega') \quad (\mathsf{KMS})$$



Papers claiming to do *without time reversal* (real boson fields):

- Carrington, Hou, Sowiak Phys. Rev. D 62, 065003 (2000)
- Wang, Heinz Phys. Rev. D 66, 025008 (2002)
- \rightarrow not correct

KMS for time reversal invariant GFs



The Single Impurity Anderson Model

$$H_{\rm imp} = \sum_{\sigma} \epsilon_{\sigma} n_{\sigma} + U(n_{\uparrow} - \frac{1}{2})(n_{\downarrow} - \frac{1}{2})$$
$$= \sum_{\sigma} (\epsilon_{\sigma} - \frac{U}{2})n_{\sigma} + Un_{\uparrow}n_{\downarrow} + c$$

$$H_{\text{leads}} = \sum_{\alpha=\mathsf{R},\mathsf{L}} \sum_{\sigma} \int dk \,\epsilon_k n_{\alpha k \sigma}$$
$$H_{\text{coup}} = \sum \int dk \, V_{\alpha k} d^{\dagger}_{\sigma} c_{\alpha k \sigma} + \text{h.c.}$$

 $\prod_{\alpha,\sigma} J$

Hybridisation function

 $\Gamma = \Gamma_{\mathsf{L}} + \Gamma_{\mathsf{R}}$

 μ_{R} μ_{L} eVGF are time reversal invariant: $G_{\sigma} = G_{\widetilde{\sigma}}|_{\widetilde{H}}$ $\Gamma_{\alpha}(\omega) = 2 \pi \sum_{k=1}^{l} \int dk |V_{\alpha k}|^2 \,\delta(\omega - \epsilon_k) \equiv \Gamma_{\alpha}$ $g_{\sigma}^{\text{Ret, Av}}(\omega) = \frac{1}{\omega - (\epsilon_{\sigma} - \frac{U}{2}) \pm i\Gamma/(2)}$

 $g^{\mathsf{K}}_{\sigma}(\omega) \ = \ F(\omega) \left[g^{\mathsf{Av}}(\omega) - g^{\mathsf{Ret}}(\omega) \right]$

$$F(\omega) = \sum_{\alpha} \frac{\Gamma_{\alpha}}{\Gamma} \left[2f_{\alpha}(\omega) - 1 \right]$$

Hybridisation as flow parameter



Flow equations and channels



Simplest freq. depend. approximation: Keep only one channel.

Example: only xph-channel
$$\dot{\gamma}(1'2'|12) = \frac{1'}{2}$$

 \rightarrow yields RPA:

$$\begin{array}{ll} \text{at } \Lambda = 0: \quad \gamma_{\sigma\bar{\sigma}|\sigma\bar{\sigma}}^{12|22}(X) \ = \ \frac{U}{2} \ - \ i \ \frac{U^2}{2\pi} \ \underbrace{\frac{1}{X - i(\frac{\Gamma}{2} - \frac{U}{\pi})}}_{\text{singularity for } U = \frac{\pi}{2}\Gamma \end{array} + \mathcal{O}\big[\big(\frac{X}{\Gamma}\big)^2\big] \\ \end{array}$$

Minimal coupling of channels



• Each channel feeds into flow of other channels as constant (renormalising the interaction)

$$\gamma(\Omega, \Delta, X) = \bar{v} + \phi_{\mathsf{pp}}(\Omega) + \phi_{\mathsf{dph}}(\Delta) + \phi_{\mathsf{xph}}(X)$$

$$\dot{\gamma}(\Omega, \Delta, X) = \dot{\phi}_{\sf pp}(\Omega) + \dot{\phi}_{\sf dph}(\Delta) + \dot{\phi}_{\sf xph}(X)$$



Minimal coupling scheme respects causality relations and KMS



Results – spectrum and effective mass



Results – linear conductance



Results – differential conductance



Results – differential conductance



Conclusion

- Approximations to frequency dependent vertex functions should respect
 - causal properties (analyticity)
 - KMS-relations (in equilibrium)
- Γ -flow can be designed to do so –
- SIAM can be treated by our Keldysh-fRG for $U \lesssim 3\Gamma$
- Justification for truncation scheme unclear

Collaborators

Mikhail Pletyukhov, Herbert Schoeller

Thanks for discussions:

Volker Meden, Christoph Karrasch, Frank Reininghaus, Sabine Andergassen, Tilman Enss, Enke Wang, Ulrich Heinz

Thanks for data:

Theo Costi, Frithjof Anders

Properties:

- Easy initial conditions
- Does not manipulate particle distribution \rightarrow compatible with KMS, respects sum rule (SIAM)
- for static fRG in equilibrium (flowing $\epsilon_{\Lambda}, U_{\Lambda}$): identical flow equations as Matsubara fRG (SIAM)
- In case of log-divergencies: regularises

$$\sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}})}{\epsilon_{\mathbf{k}} - \omega + i\eta} \sim \log \frac{\max\{T, |\omega - \mu|, \eta\}}{D}$$

- Flow equation does not replace one summation/integration
 - \rightarrow higher numerical effort