

# Fermionic functional renormalization group for first-order phase transitions

*A mean-field model*

Roland Gersch, Julius Reiss, Carsten Honerkamp

Dept. Metzner, MPI for Solid State Research, Stuttgart



für Festkörperforschung

Dresden, 27.02.2007

The fRG can scan a system's order parameter space for minima of the thermodynamic potential.

1. Some fRG
2. Bias as a challenge
3. Bias as a chance

- Spontaneous symmetry breaking

$$\sum_X \Psi_X \mathbb{Q}(X) \Psi_X \xrightarrow{\text{i.a.}} \sum_{XY} \Psi_X (\mathbb{Q}(X) - \Delta(X, Y)) \Psi_Y$$

- Microscopic models  $\xrightarrow{\text{fRG}}$  physical observables
- Fermionic degrees of freedom kept
- Unbiased approach for multiple instabilities  
Zanchi and Schulz 1998, Halboth and Metzner 2000, Salmhofer, Honerkamp, Furukawa, Rice 2001, Metzner, Reiss, Rohe 2005, Dupuis 2005.
- Rigorous error estimates available  
Salmhofer, Honerkamp 2001

# Formalities

- Generating functional of connected Green's functions

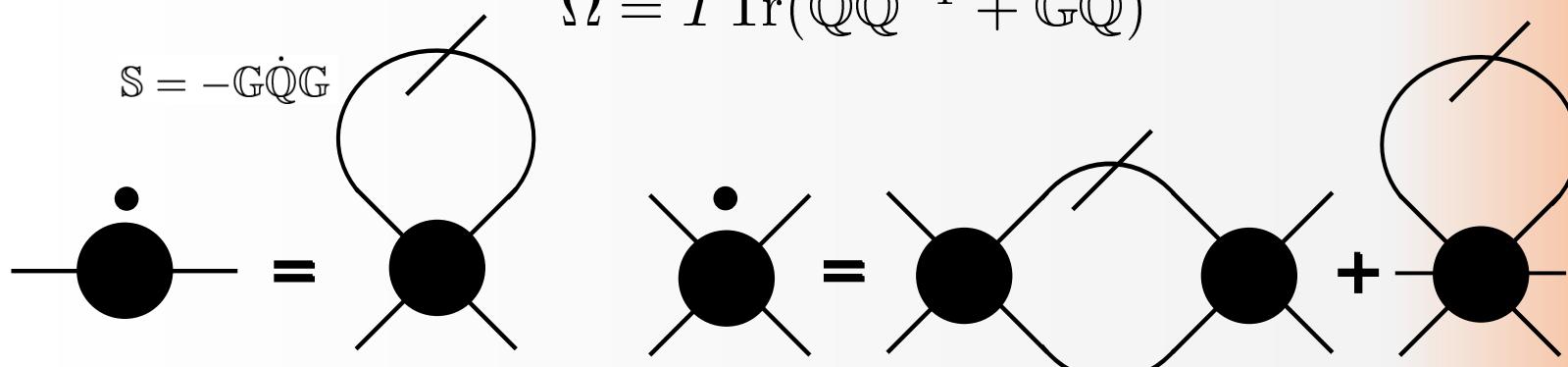
$$\exp(-W(J)) = \int \frac{\mathcal{D}\Psi}{\det \mathbb{Q}/\chi(\Lambda)} e^{(\Psi, \mathbb{Q}/\chi(\Lambda)\Psi) - V(\Psi) + (J, \Psi)}$$

$J$ : Grassmannian generating field,  $V$ : two-particle interaction

- $\chi(\Lambda_i)$  makes  $W$  solvable,  $\chi(\Lambda_f) \equiv 1$ .

One-particle irreducible (1PI) flow Salmhofer, Honerkamp 2001

$$\dot{\Omega} = T \text{Tr}(\dot{\mathbb{Q}} \mathbb{Q}^{-1} + \mathbb{G} \dot{\mathbb{Q}})$$



# Formalities

- Generating functional of connected Green's functions

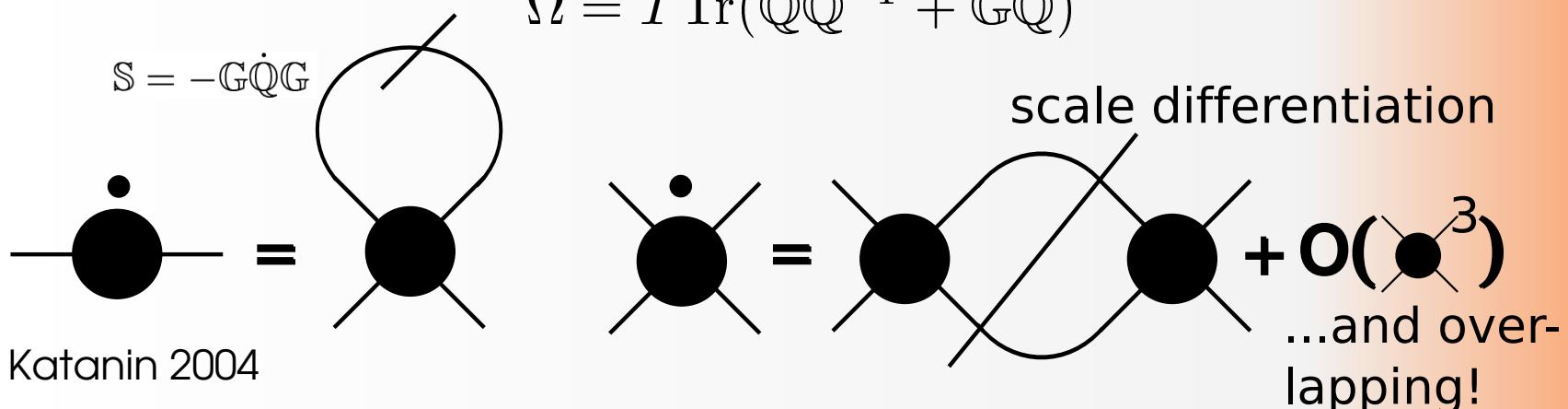
$$\exp(-W(J)) = \int \frac{\mathcal{D}\Psi}{\det \mathbb{Q}/\chi(\Lambda)} e^{(\Psi, \mathbb{Q}/\chi(\Lambda)\Psi) - V(\Psi) + (J, \Psi)}$$

$J$ : Grassmannian generating field,  $V$ : two-particle interaction

- $\chi(\Lambda_i)$  makes  $W$  solvable,  $\chi(\Lambda_f) \equiv 1$ .

One-particle irreducible (1PI) flow Salmhofer, Honerkamp 2001

$$\dot{\Omega} = T \text{Tr}(\dot{\mathbb{Q}} \mathbb{Q}^{-1} + \mathbb{G} \dot{\mathbb{Q}})$$



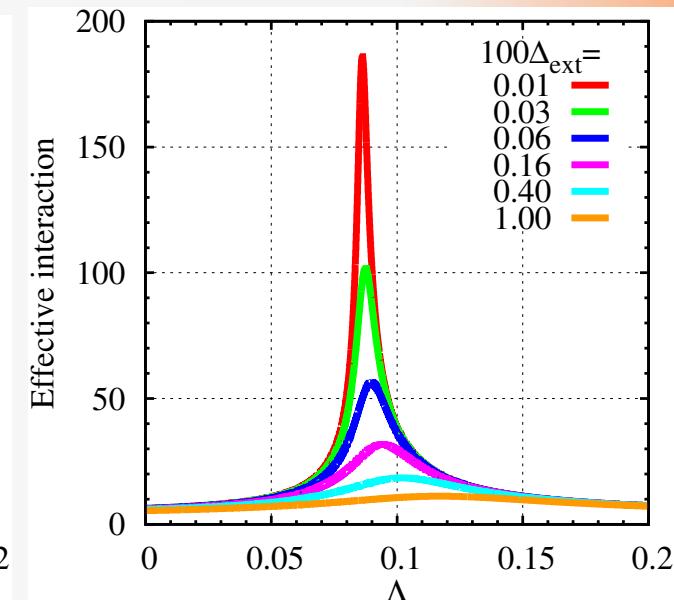
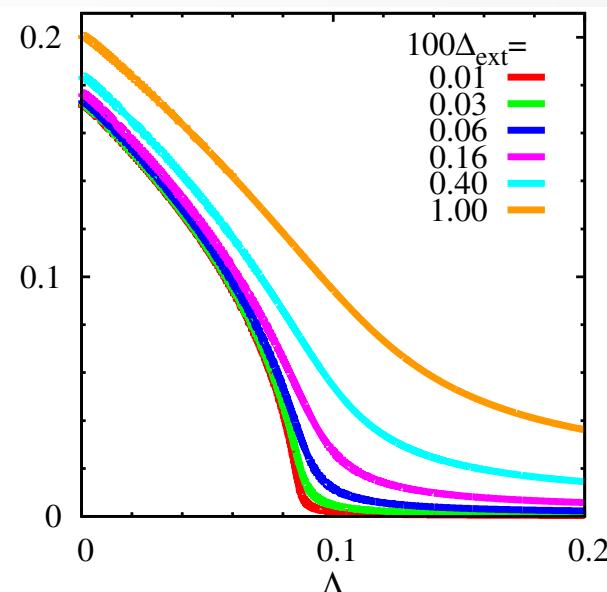
# The external field's influence

Charge-density-wave mean-field model Hamiltonian

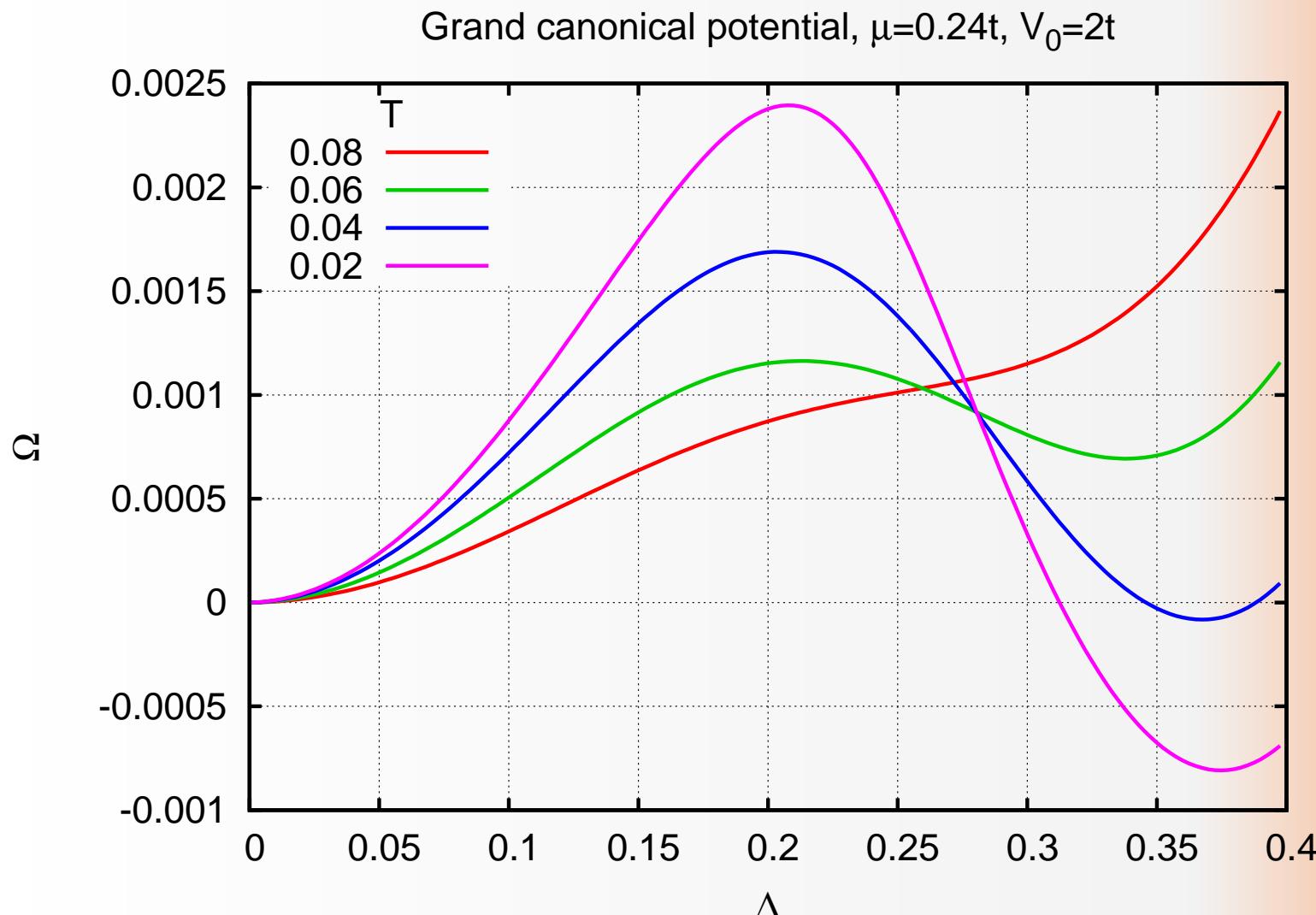
$$H = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}}^\dagger c_{\mathbf{k}} - \frac{V_0}{N} \sum_{\mathbf{k}, \mathbf{k}'} c_{\mathbf{k}}^\dagger c_{\mathbf{k}+\mathbf{Q}} c_{\mathbf{k}'}^\dagger c_{\mathbf{k}'+\mathbf{Q}}$$
$$+ \sum_{\mathbf{k}} (\Delta_c - \Delta_i) c_{\mathbf{k}+\mathbf{Q}}^\dagger c_{\mathbf{k}}, \quad \mathbf{Q} = (\pi, \pi, \dots)$$

$\mu$ : chemical potential,  $\varepsilon$ : tight-binding dispersion,  $V_0$ : nearest-neighbor repulsion,  $\Delta_c - \Delta_i$ : external field.

$T = \mu = 0$  :  
RG, Honer-  
kamp, Rohe, ▲  
Metzner 2005  
Units: hopping  
integral



# First-order phase transitions



# Counterterms: first attempt

- Back to the CDW Hamiltonian.

$$H = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}}^\dagger c_{\mathbf{k}} - \frac{V_0}{N} \sum_{\mathbf{k}, \mathbf{k}'} c_{\mathbf{k}}^\dagger c_{\mathbf{k}+\mathbf{Q}} c_{\mathbf{k}'}^\dagger c_{\mathbf{k}'+\mathbf{Q}}$$

$$+ \sum_{\mathbf{k}} (\Delta_c - \Delta_i) c_{\mathbf{k}+\mathbf{Q}}^\dagger c_{\mathbf{k}}$$

- To bare propagator
- To initial self-energy

$$\mathbb{G}^{-1} = \frac{1}{\chi} \begin{pmatrix} i\omega - \varepsilon + \mu & \Delta_c - \chi\Delta \\ \Delta_c - \chi\Delta & i\omega + \varepsilon + \mu \end{pmatrix}$$

$$\Rightarrow \mathbb{G}_{12} \propto \chi \cdot \underbrace{(\chi\Delta - \Delta_c)}_{=:-\Delta_{\text{eff}}} \stackrel{\chi(\Lambda) \in \{0,1\}}{\Rightarrow} \dot{\Delta} = \text{Diagram} \propto \chi \cdot (\chi\Delta - \Delta_c) = 0$$

$\chi(\Lambda) \equiv \sqrt{\Lambda}$ ,  $\Lambda_i = 0$ ,  $\Lambda_f = 1$  equivalent to linearly turning on the interaction from 0 to  $V_0$ .

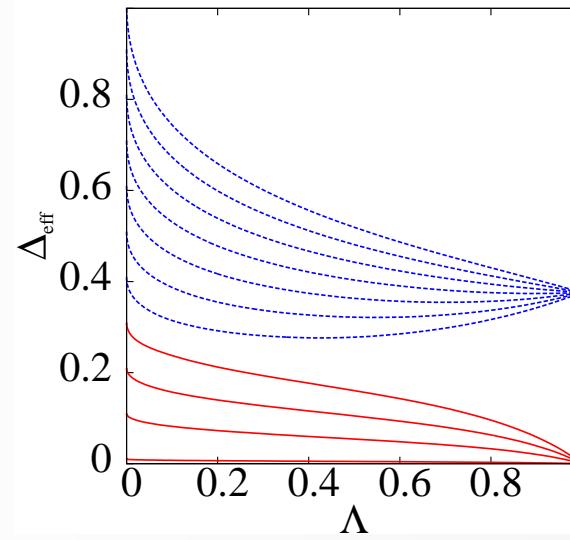
Honerkamp, Rohe, Andergassen, Enss 2004.

*Advantages:*

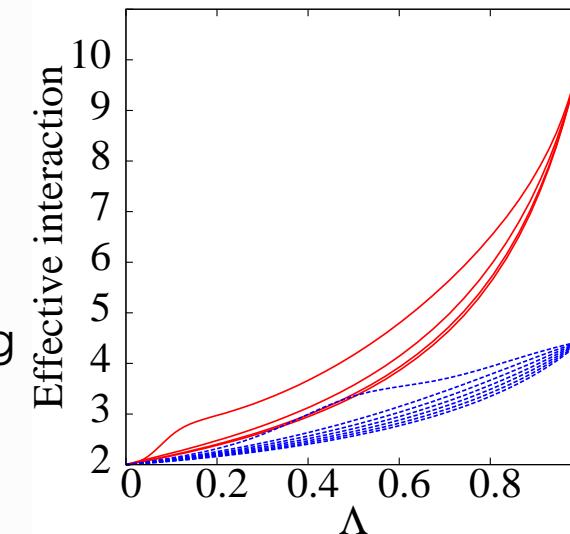
- $\chi\Delta_{\text{eff}}|_{\Lambda=\delta\Lambda} \approx \sqrt{\delta\Lambda}(-\Delta_c) \neq 0$
- Thus,  $\dot{\Delta} \neq 0$ .
- Chosing  $\Delta_i = \Delta_c$ : scanning the order parameter space for thermodynamic potential minima.
- Results independent of  $\Delta_i$  for mean-field models
- Large effective interactions restricted to the final region of the flow

# First-order CDW phase transition

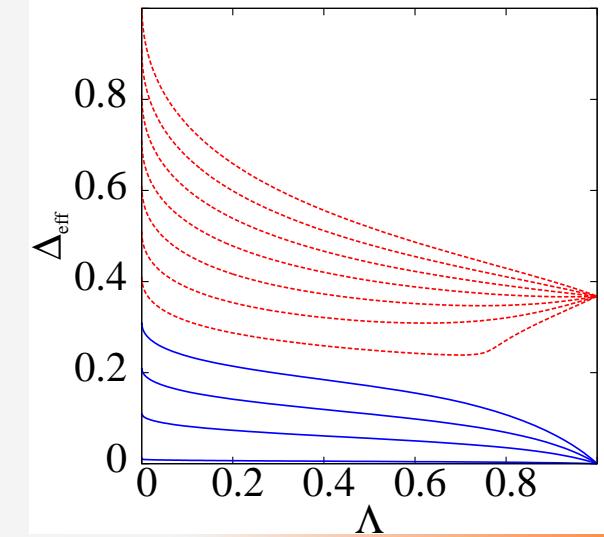
Order parameter  
 $T < T_t$   
units: hopping integral



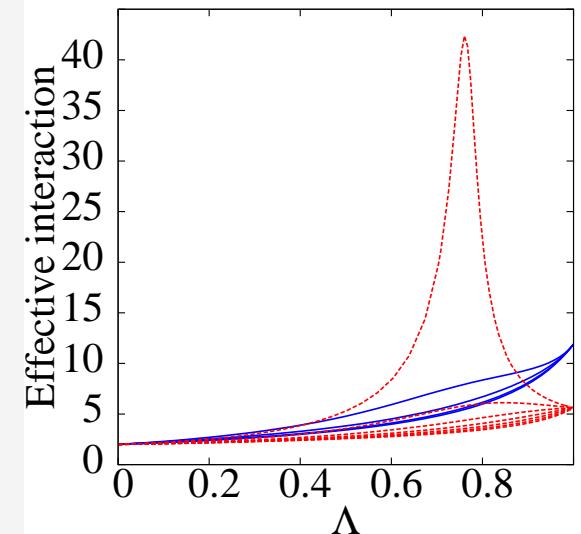
Effective interaction  
 $T < T_t$   
units: hopping integral



$T > T_t$



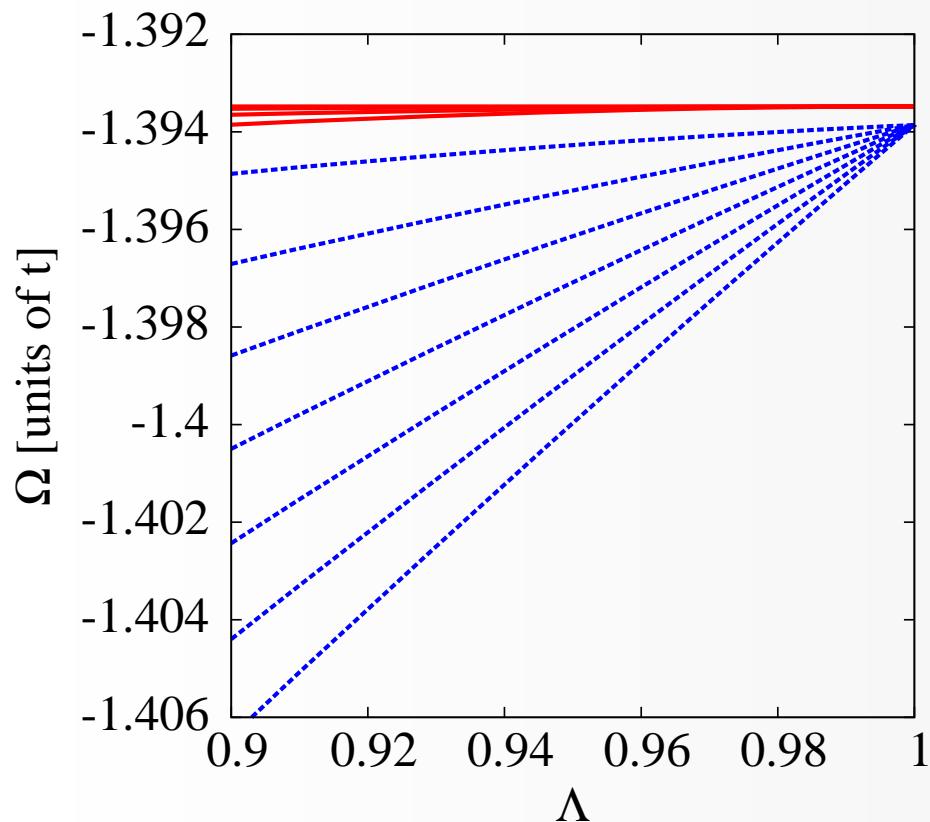
$T > T_t$



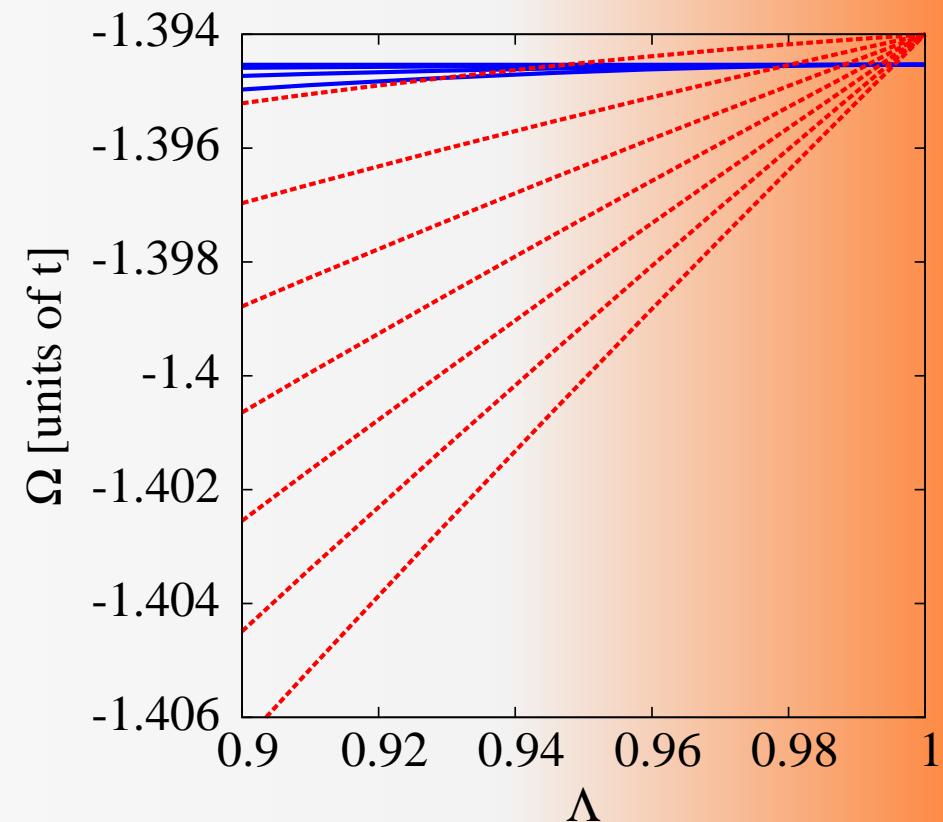
RG, Reiss, Honerkamp 2006

# Flow of $\Omega$

$\Omega$  for  $T < T_t$ :



$\Omega$  for  $T > T_t$ :



RG, Reiss, Honerkamp 2006



# Conclusions

- The fRG is set up as a powerful tool for the study of symmetry breaking.
- A method to study stable and metastable states has been developed. Bias has turned from challenge to chance.
- Studies of models with extended momentum structure remain to be done (discretization: patching, expansion, ...?)

Thank you very much!

