First-order phase transitions with the Katanin scheme

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für Festkörperforschung

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Message

The fermionic fRG (f^2RG) can cope with first-order phase transitions.

(and it's not so hard)

More subtly put:

The f^2RG can scan a system's order parameter space for minima of the thermodynamic potential.

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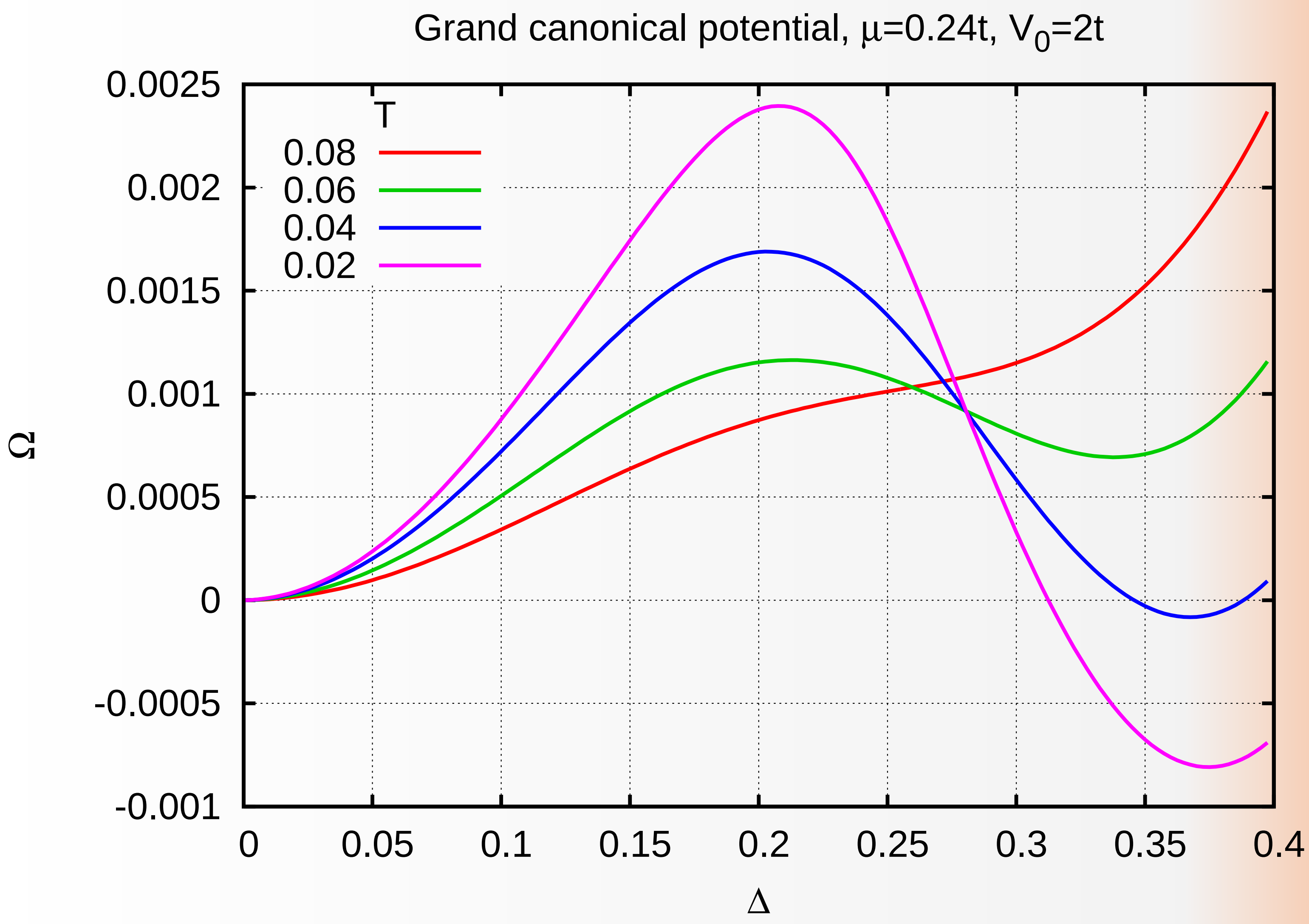
Thermodynamic potential and phases



Hamiltonian

- At half-filling: a repulsive interaction restricted to momentum-transfers of $\mathbf{Q} := (\pi, \pi, \dots)$ generates a d-dimensional charge-density wave.

$$H = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) c^\dagger_{\mathbf{k}} c_{\mathbf{k}} - \frac{V_0}{N} \sum_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}} c_{\mathbf{k}+\mathbf{Q}} c^\dagger_{\mathbf{k}'} c_{\mathbf{k}'+\mathbf{Q}} + \sum_{\mathbf{k}} (\Delta_{\mathrm{c}} - \Sigma_{\mathrm{i}}) c^\dagger_{\mathbf{k}+\mathbf{Q}} c_{\mathbf{k}}$$

- For certain parameters, the lattice translation symmetry (which is discrete) will be broken.

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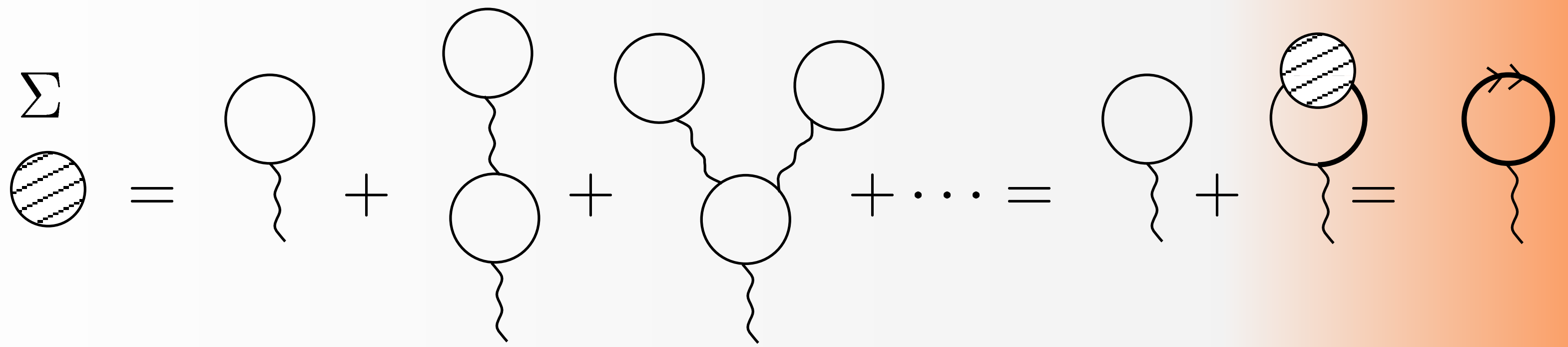
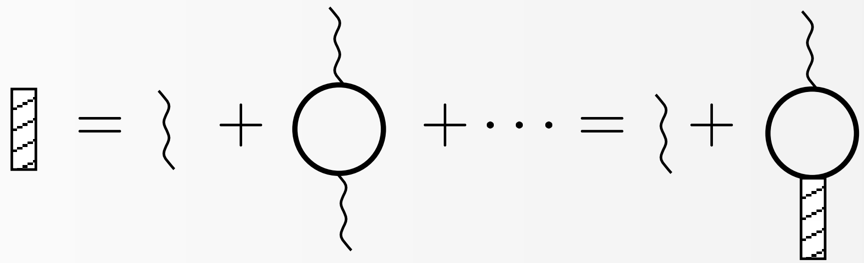
Mean-field-exact toy model

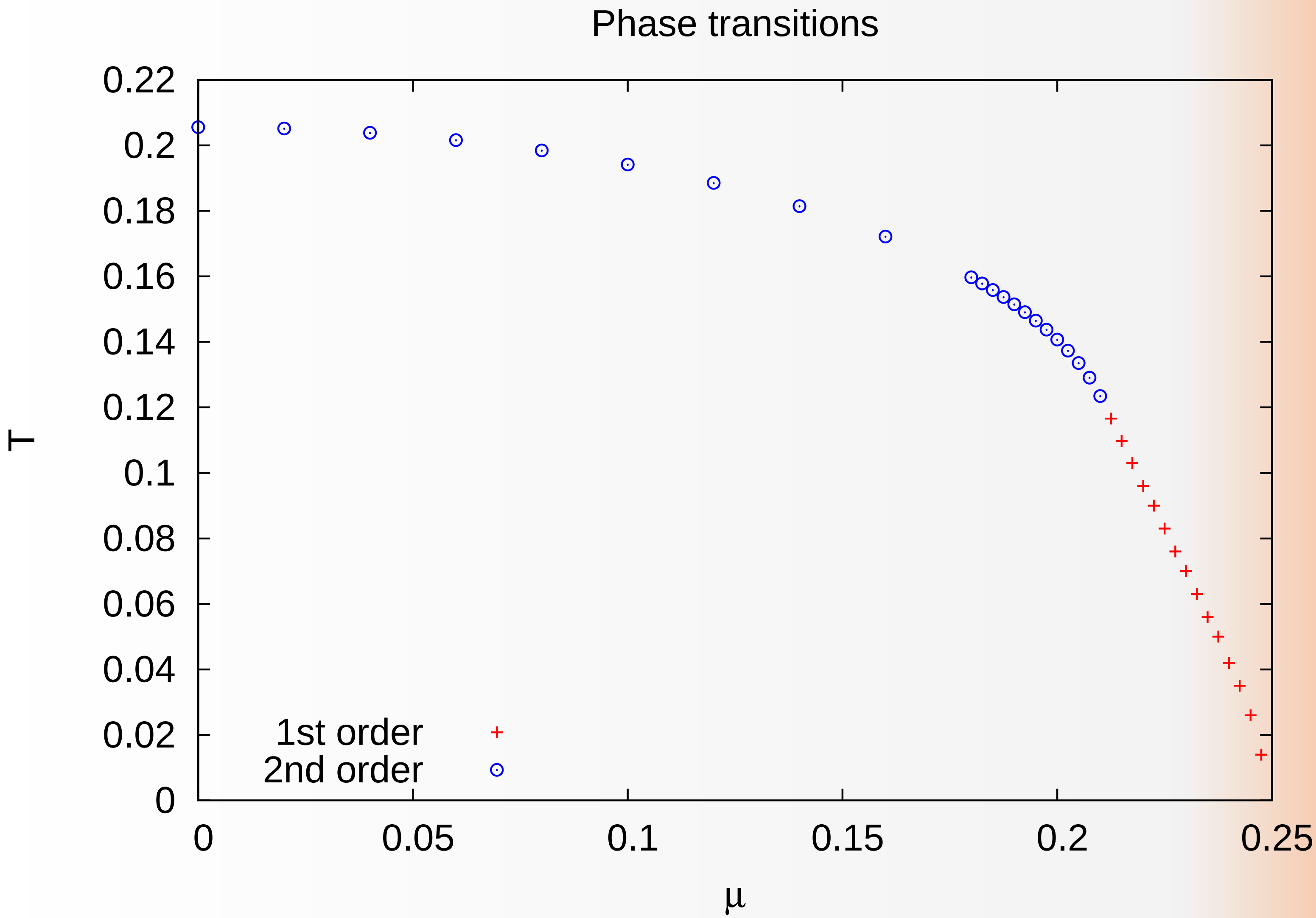
- Resumming perturbation theory ⇒ gap equation.



- RPA resummation for effective interaction
  ⇒ Bethe-Salpeter equation.

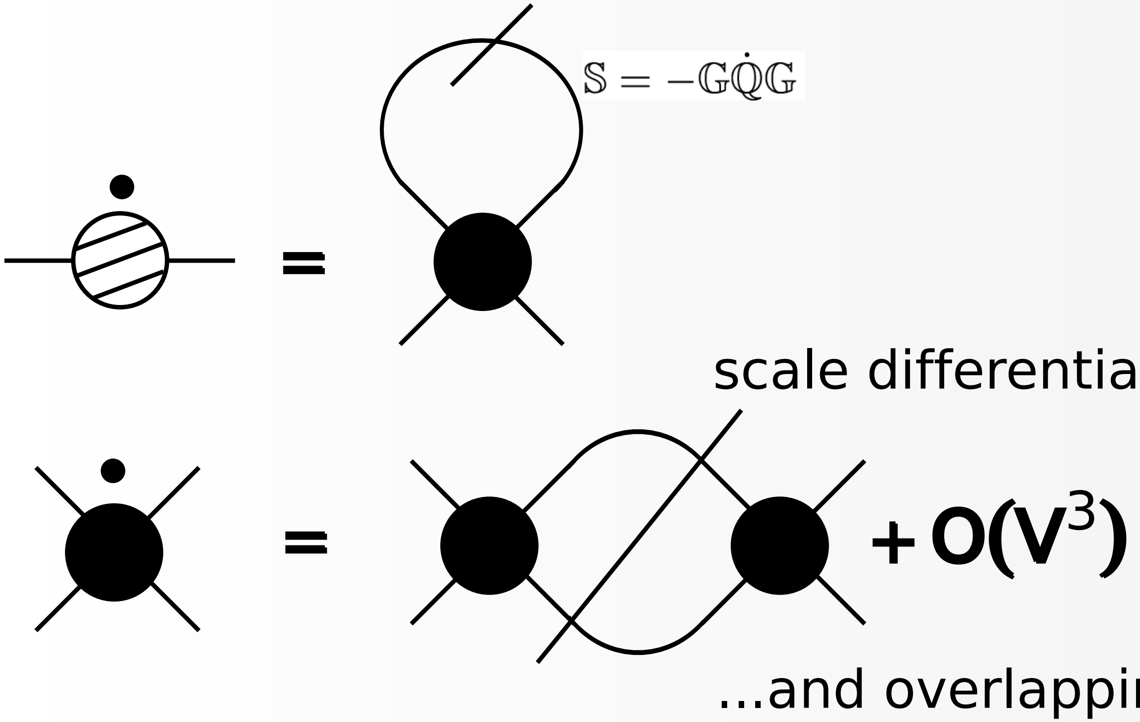


Phase diagram



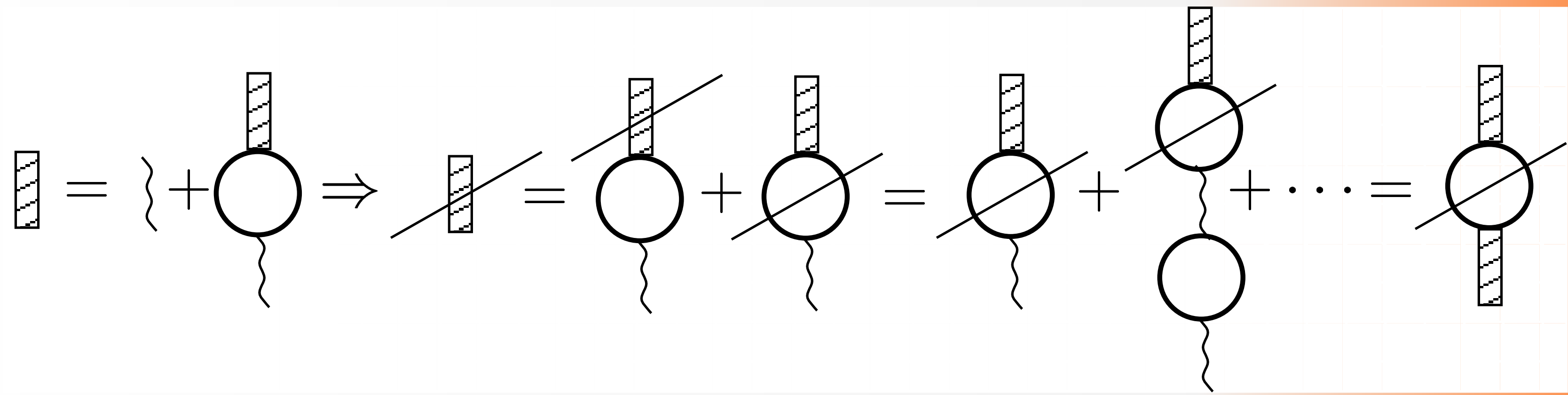
One-particle irreducible (1PI) scheme

Introduce cutoff Λ, cutoff function $\chi(\Lambda)$: $\mathbb{G}_0^{-1} \to \mathbb{G}_0^{-1}/\chi =: \mathbb{Q}$

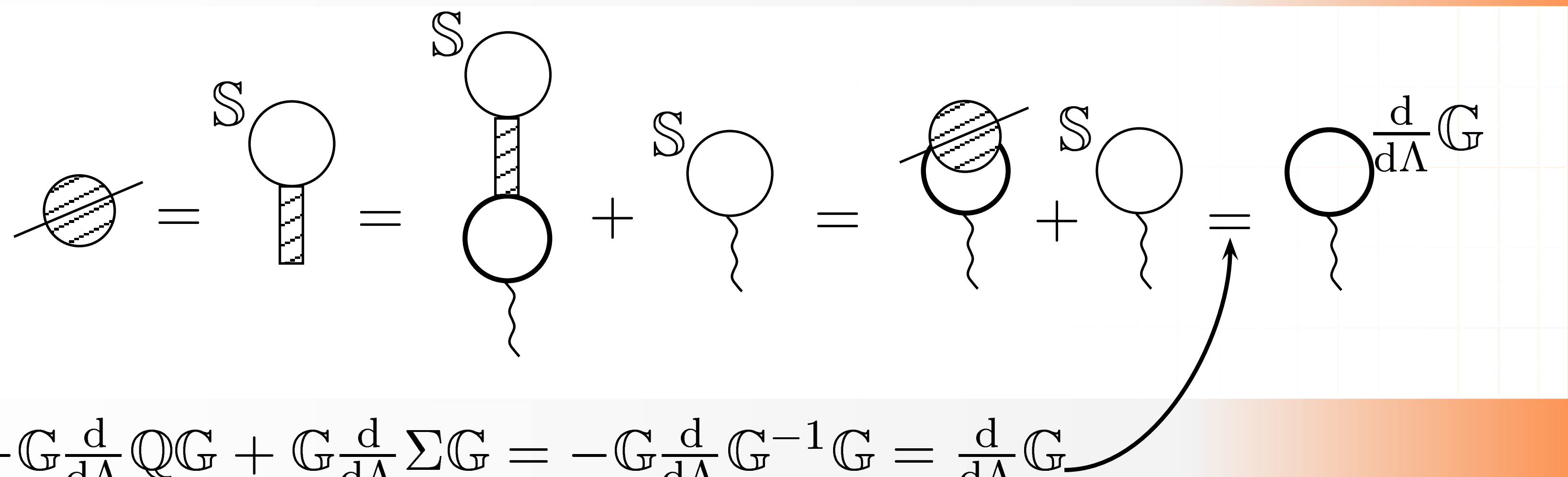


f^2RG equations

- Vertex flow equation from Bethe-Salpeter equation:

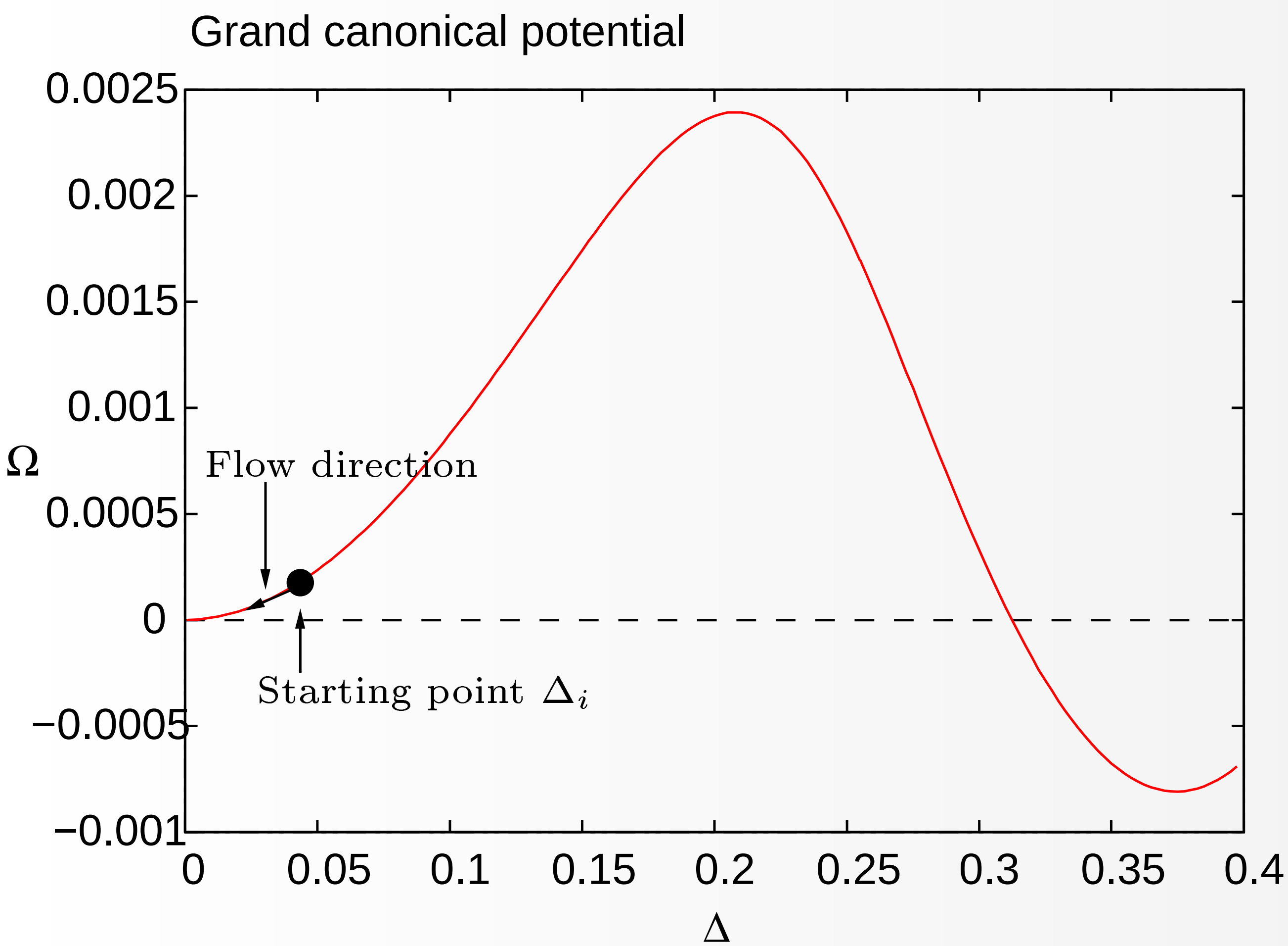


- Gap equation from gap flow equation: $\mathbb{S} := -\mathbb{G}\dot{\mathbb{Q}}\mathbb{G}$:



$$-\mathbb{G}\frac{\mathrm{d}}{\mathrm{d}\Lambda}\mathbb{Q}\mathbb{G} + \mathbb{G}\frac{\mathrm{d}}{\mathrm{d}\Lambda}\Sigma\mathbb{G} = -\mathbb{G}\frac{\mathrm{d}}{\mathrm{d}\Lambda}\mathbb{G}^{-1}\mathbb{G} = \frac{\mathrm{d}}{\mathrm{d}\Lambda}\mathbb{G}$$

Challenge



Challenge: Starting at large Δ *without* appreciably changing $\Omega(\Delta)$.

Counter terms and interaction flow

- Back to the Hamiltonian.

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

$$+ \sum_{\mathbf{k}} (\Delta_{\mathrm{c}} - \Sigma_{\mathrm{i}}) c^{\dagger}_{\mathbf{k}+\mathbf{Q}} c_{\mathbf{k}}$$

- To naked propagator
- To initial self-energy

$$\mathbb{G}^{-1} = \frac{1}{\chi}\left(\mathbb{Q} + \Delta_{\mathrm{c}}\sigma_x - \chi\Sigma\sigma_x\right) \Rightarrow$$

$$\mathbb{G}_{12} \propto \chi \cdot (\underbrace{\chi\Sigma - \Delta_{\mathrm{c}}}_{=:-\Delta_{\mathrm{f}}})$$

- $\chi = \Theta(\varepsilon_k - \mu - \Lambda)$: Σ and Δ_{c} cancel at all scales.
- $\chi = \sqrt{\Lambda}$: Σ_{i} and Δ_{c} cancel *only* at the end of the flow. The initial self-energy can be chosen arbitrarily without changing the physics!

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Grand canonical potential flow

$$\dot{\Omega} = \frac{T}{2}\mathrm{Tr}\left(\left(\mathbb{G} - \mathbb{Q}^{-1}\right)\dot{\mathbb{Q}}\right)$$

$$= -\frac{T}{2}\mathrm{Tr}\left(\left(\mathbb{Q}^{-1}\sum_n(\Sigma\mathbb{Q}^{-1})^n - \mathbb{Q}^{-1}\right)\mathbb{Q}\frac{\dot{\chi}}{\chi}\right)$$

$$= -\frac{T}{2}\mathrm{Tr}\left(\sum_{n=1}(\Sigma\mathbb{Q}^{-1})^n\frac{\dot{\chi}}{\chi}\right)$$

$$= -\frac{T}{2}\mathrm{Tr}\left(\Sigma\sum_n(\mathbb{Q}^{-1}\Sigma)^n\mathbb{Q}^{-1}\frac{\dot{\chi}}{\chi}\right)$$

$$= -\frac{T}{2}\mathrm{Tr}\left(\Sigma\mathbb{G}\frac{\dot{\chi}}{\chi}\right)$$

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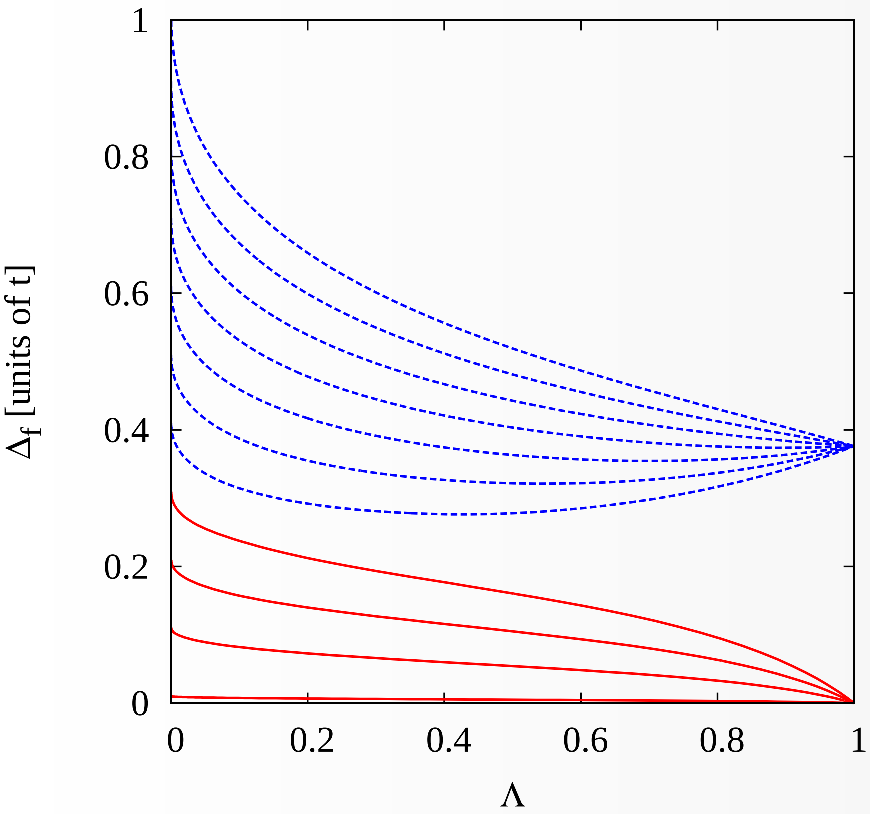
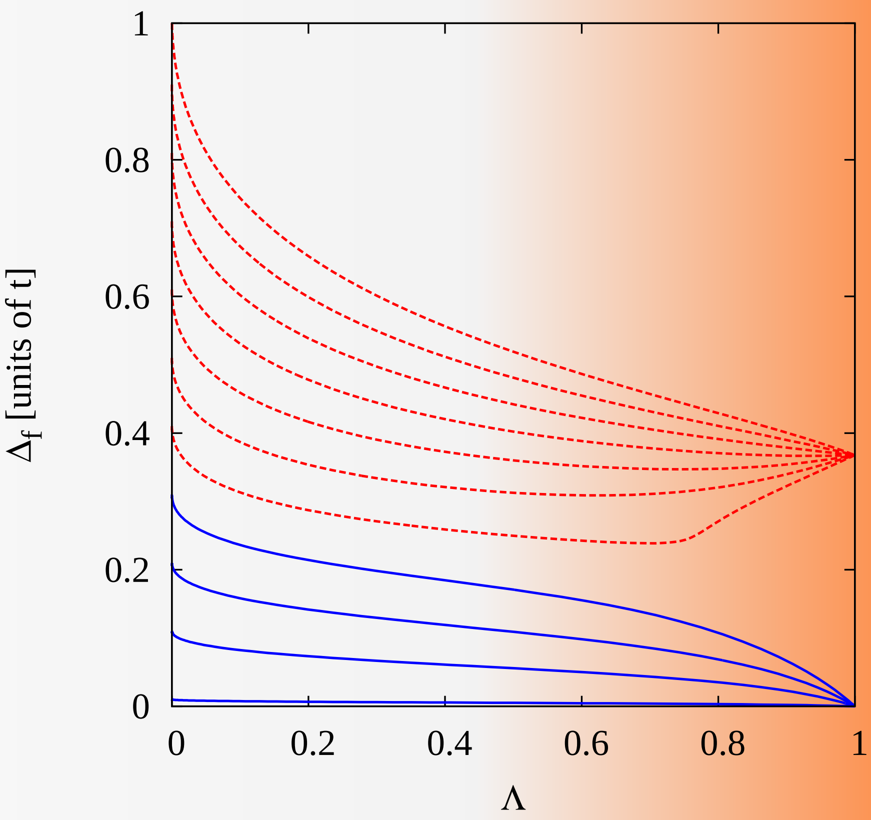
Numerical results: Σ

Σ for $T < T_t$:



Σ for $T > T_t$:



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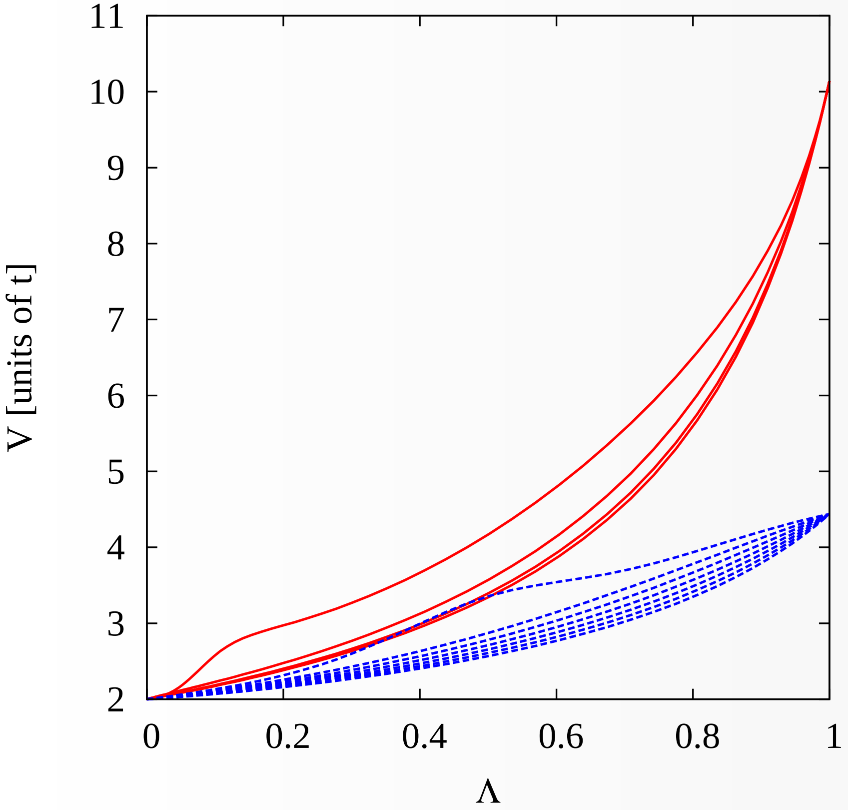
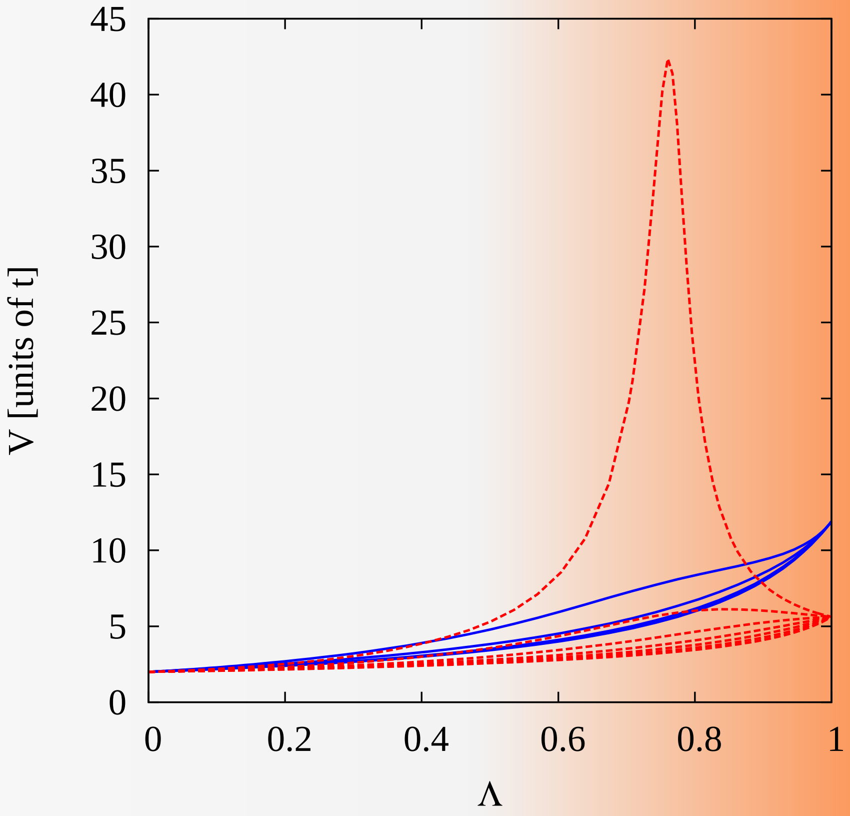
Numerical results: V

V for $T < T_t$:



V for $T > T_t$:



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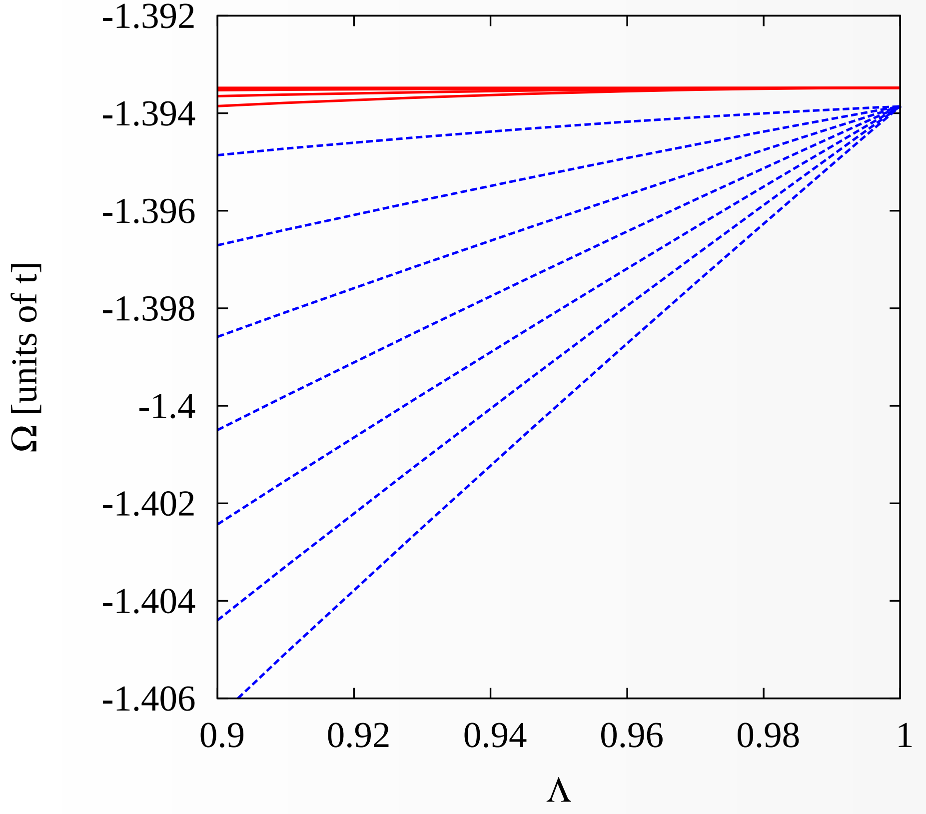
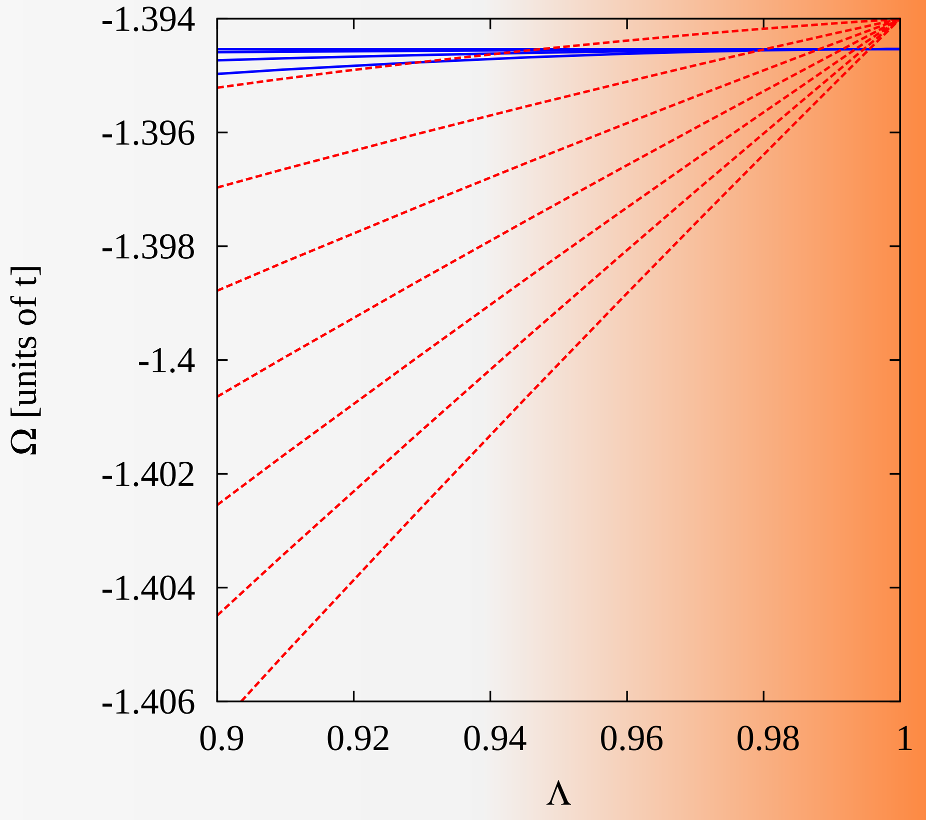
Numerical results: Ω

Ω for $T < T_t$:



Ω for $T > T_t$:



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Conclusion & Outlook

1. The f^2RG can scan a system's order parameter space for minima of the thermodynamic potential.
2. The f^2RG can do first-order phase transitions.
3. Katanin's scheme reproduces mean-field exactly.

We need to treat full models!

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