The crossover from Fermi liquid to local pairs in the normal state of the attractive Hubbard and Holstein models

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Collaborations

Pairing and polarization

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Divergent precursors of Mott transition

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G. Rohringer

O. Gunnarsson

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A. Toschi

PHYSICAL REVIEW B **73**, 245114 (2006)

Pairing and polarization in electron-boson systems with retarded interactions via dynamical mean-field theory

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Divergent Precursors of the Mott-Hubbard Transition at the Two-Particle Level

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- Introduction
- Polarization crossover
  - Holstein model, polarization, bipolarons
  - The classical limit of the Holstein model, polarization crossover
- Pairing crossover
  - The negative U limit of the Holstein model
  - The “centroid” variable
  - Pairing in the Holstein and attractive Hubbard model
  - FDT for centroids
- Negative & positive U
  - Spin & pseudospin
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Introduction

- BCS to Bose-Einstein crossover → Pairing
- Polaron crossover → Polarization

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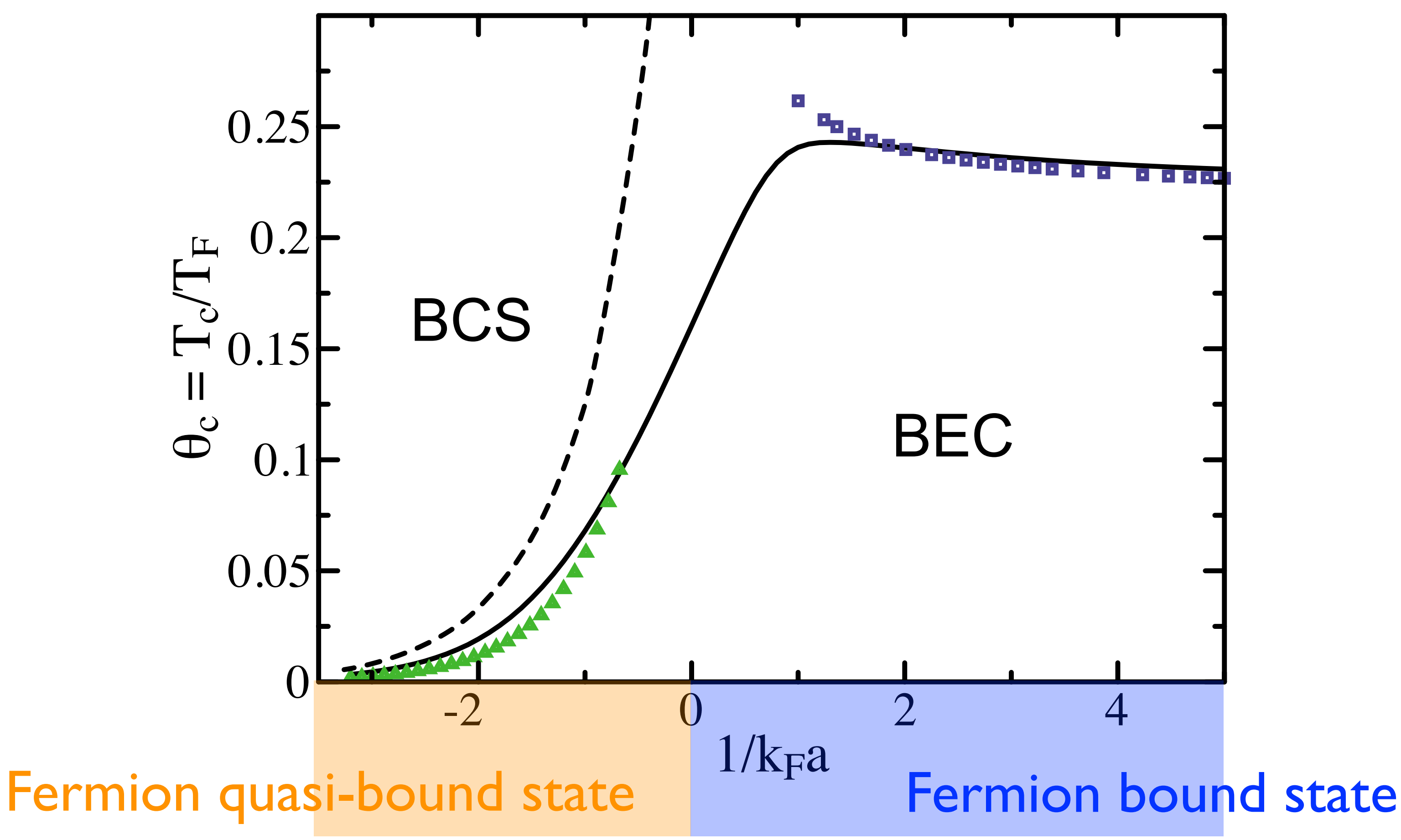
BEC in ultracold gases



[I.Bloch J.Dalibard W.Zwerger Rev. Mod. Phys. 80, 885 (2008)]

Introduction

- BCS to Bose-Einstein crossover → Pairing
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Polaron crossover in magnanites

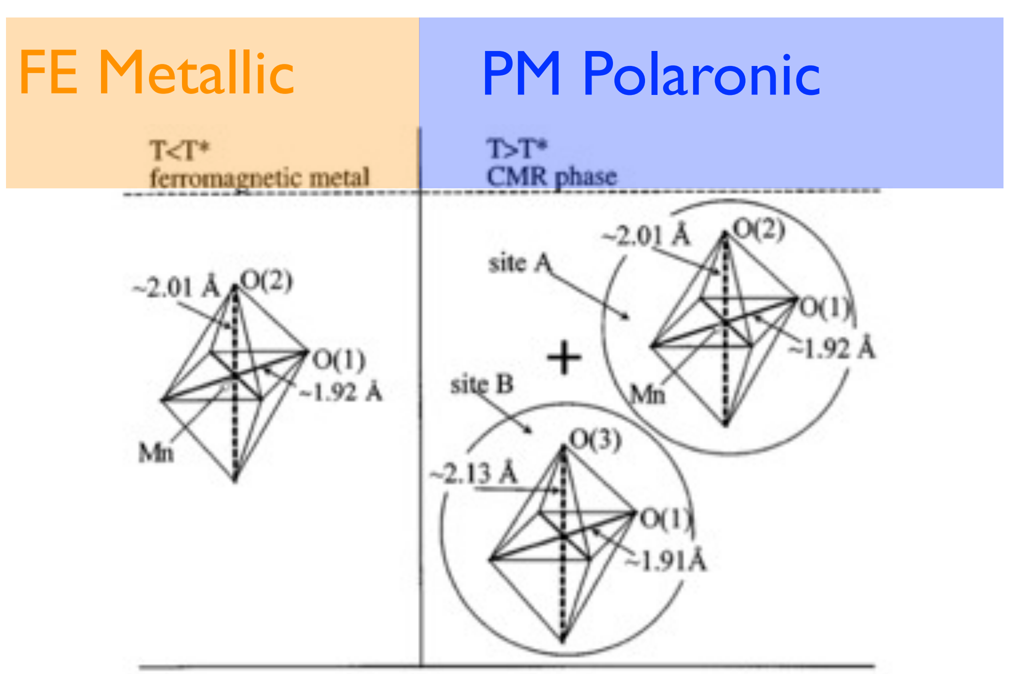
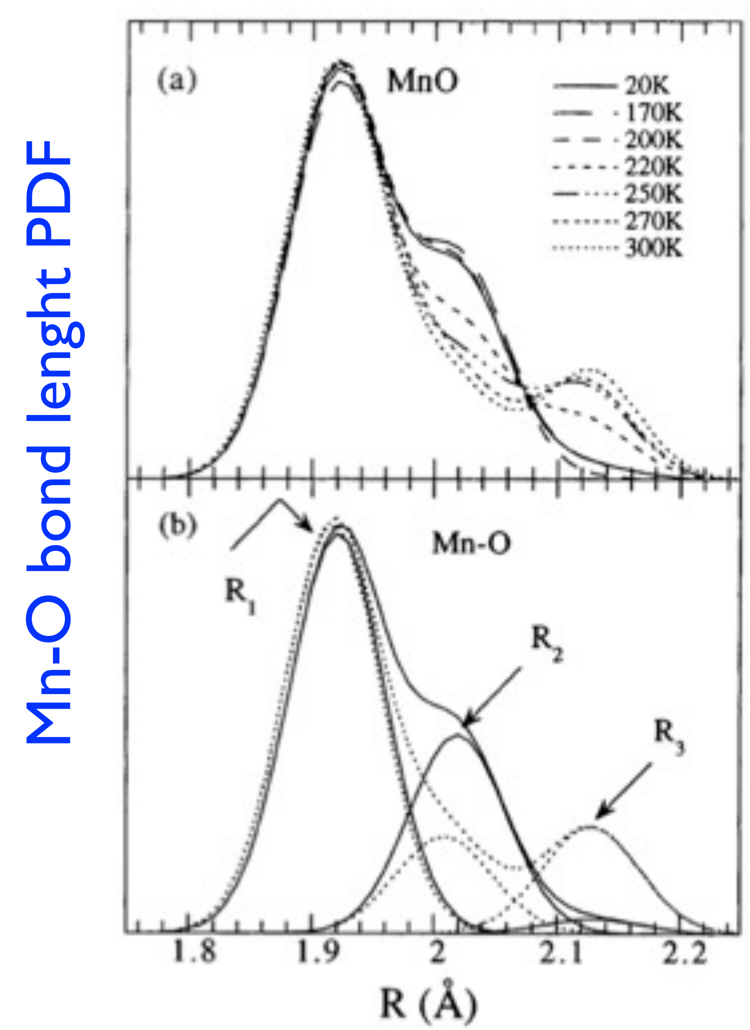


FIG. 4. Pictorical view of the MnO_6 octahedral local distortions in the metallic and insulating phase.

[A.Lanzara et al. PRL 81, 878 (1998)]

$La_{0.75}Ca_{0.25}MnO_3$



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Holstein Model

$$H = \underbrace{\omega_0 \sum_i a_i^\dagger a_i}_{H_b} \underbrace{- t \sum_{<i,j>,\sigma} c_{i,\sigma}^{+} c_{j,\sigma} - g \sum_{i,\sigma} (a_i^\dagger + a_i) c_{i,\sigma}^{+} c_{i,\sigma}}_{H_{el}}$$

Adiabatic ratio: $\gamma = \omega_0 / D$ (D=half bandwidth)

e-b coupling (adiabatic $\gamma < 1$): $\lambda = 2g^2/\omega_0 D$

e-b coupling (antiadiabatic $\gamma > 1$): $\alpha^2 = g^2/\omega_0^2$

Holstein Model: polarons & bipolarons

Atomic limit t=0

$$H = \omega_0 a^\dagger a - g \sum_\sigma (a^\dagger + a) n_\sigma$$

Density dependent displaced harmonic oscillator

lattice polarization

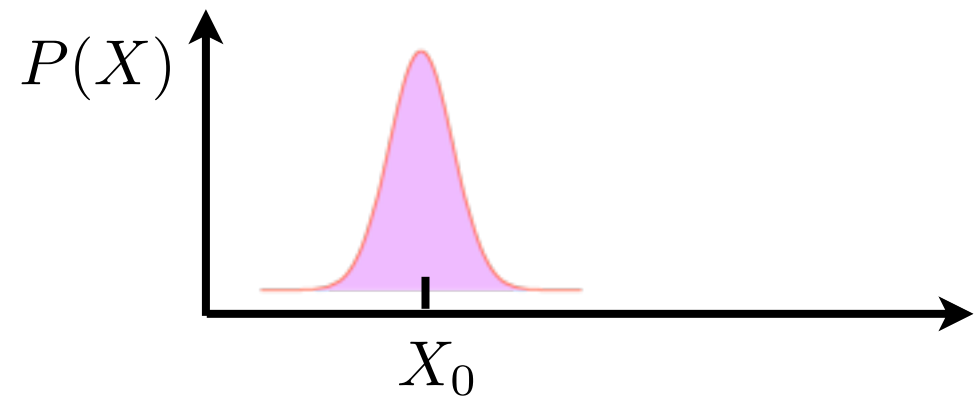
$$x = a + a^\dagger \quad P(x) =< \Psi|x >< x|\Psi >$$

Holstein Model: polarons & bipolarons

Atomic limit t=0 $H = \omega_0 a^\dagger a - g \sum_\sigma (a^\dagger + a) n_\sigma$

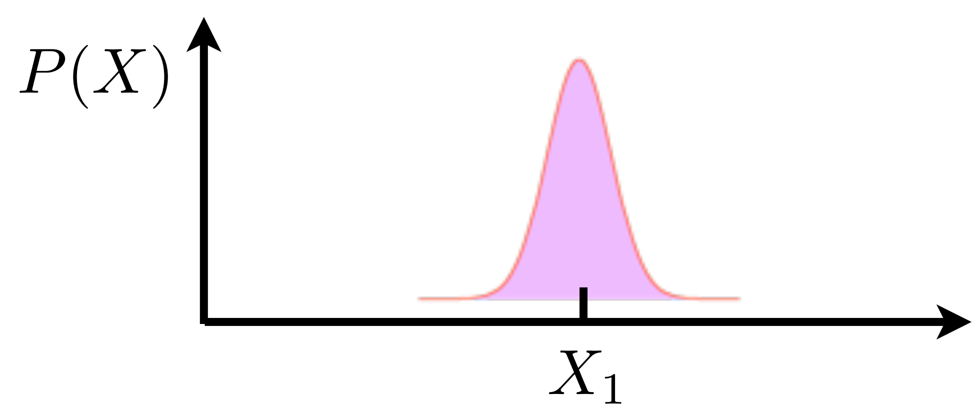
n=0 free oscillator

$$E_0 = 0$$
$$X_0 = 0$$



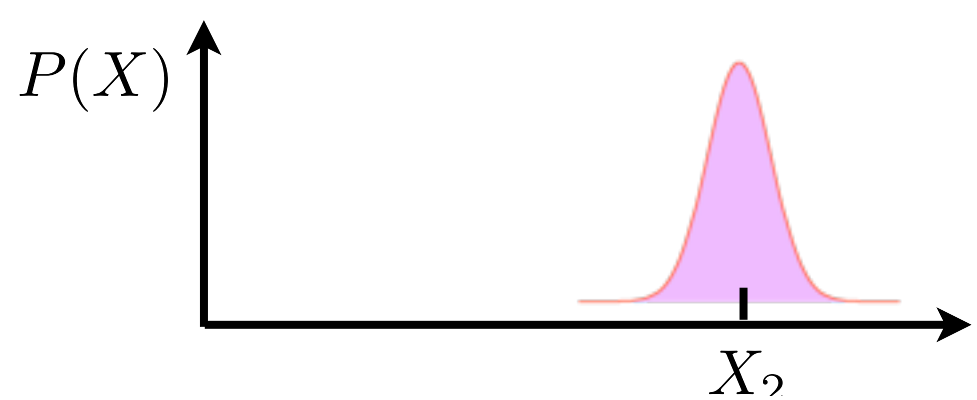
n=1 polaron

$$E_1 = -g^2/\omega_0$$
$$X_1 = 2g/\omega_0$$



n=2 bipolaron

$$E_2 = 2E_1 - 2g^2/\omega_0$$
$$X_2 = 4g/\omega_0$$



Holstein Model: polarons & bipolarons

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n=0 free oscillator

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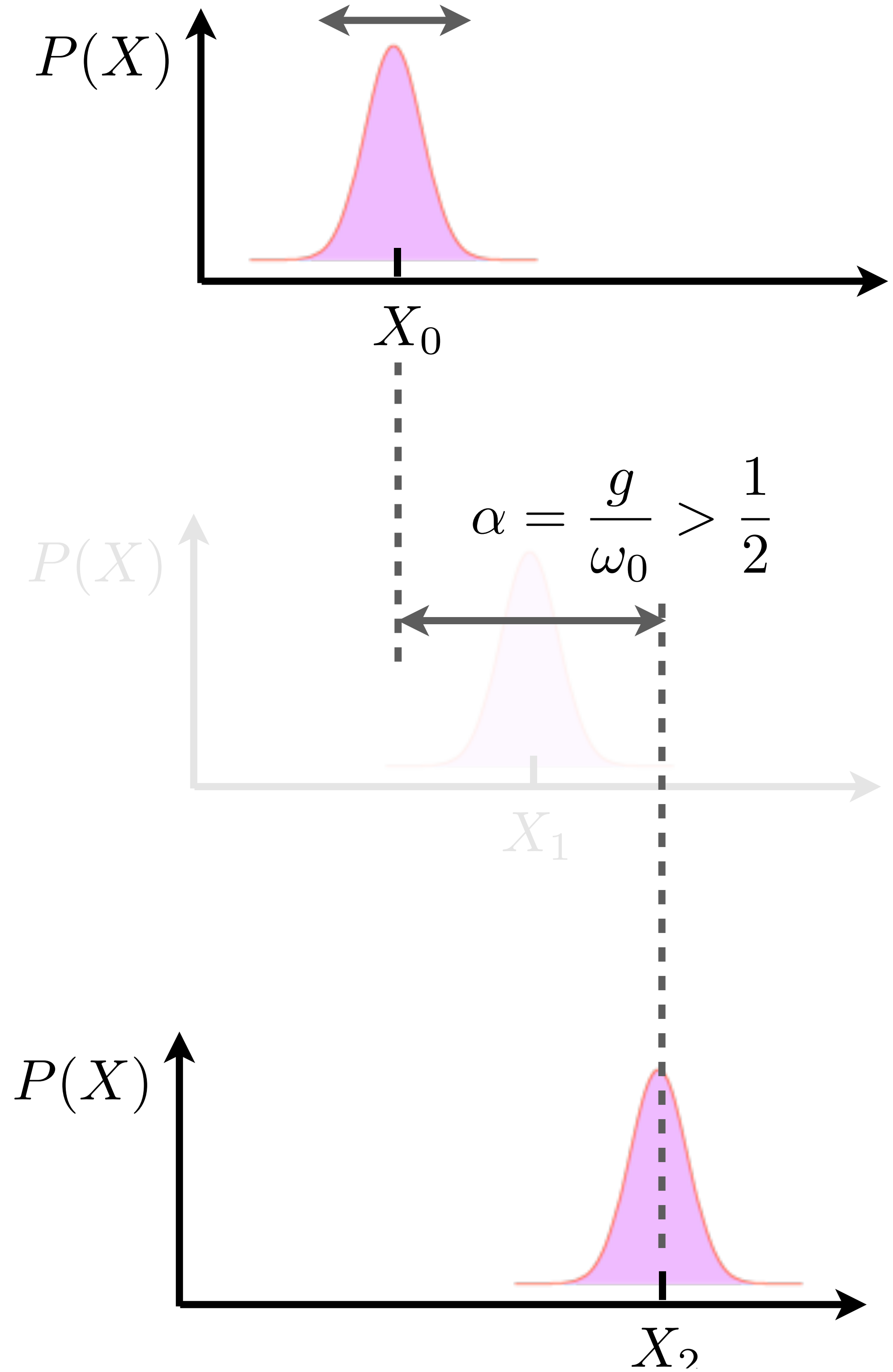

Path integral in a nutshell

$$H = \frac{P^2}{2m} + V(X)$$

$$Z = tr\ e^{-\beta H} = \int dX < X|e^{-\beta H}|X >$$

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$\left(e^{-\Delta\tau H}\right)^M \quad \Delta\tau = \beta/M$ **Trotter formula**

$$Z = \int dX \int dX_1 \cdots \int dX_M < X|e^{-\Delta\tau H}|X_1 >< X_1|e^{-\Delta\tau H}|X_2 > \cdots < X_M|e^{-\Delta\tau H}|X >$$

Path integral in a nutshell

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$$e^{-\Delta\tau H} = e^{-\Delta\tau V/2} e^{-\Delta\tau \frac{P^2}{2m}} e^{-\Delta\tau V/2} + o(\Delta\tau^2)$$ Suzuki formula

$$< X_1|e^{-\Delta\tau H}|X_2 >= e^{-\Delta\tau V(X_1)/2} < X_1|e^{-\Delta\tau \frac{P^2}{2m}}|X_2 > e^{-\Delta\tau V(X_2)/2}$$

$$< X_1|e^{-\Delta\tau \frac{P^2}{2m}}|X_2 > \propto e^{-m\frac{(X_1-X_2)^2}{2\Delta\tau}} = e^{-\frac{m}{2}\Delta\tau\left(\frac{X_1-X_2}{\Delta\tau}\right)^2}$$

Path integral in a nutshell

$$H = \frac{P^2}{2m} + V(X)$$

$$Z \propto \int dX \int dX_1 \cdots \int dX_M e^{-S}$$

$$S = \sum_{i=1,M+1} \Delta\tau \left[\frac{1}{2} m \left(\frac{X_i - X_{i-1}}{\Delta\tau} \right)^2 + V(X_i) \right] \qquad \begin{aligned} X_0 &= X \\ X_{M+1} &= X \end{aligned}$$

Kinetic Potential

Path integral in a nutshell

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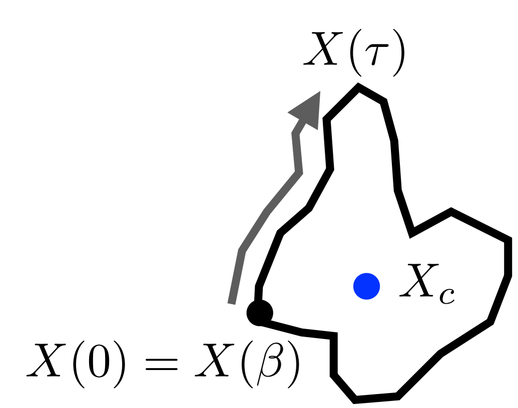
Kinetic Potential

$$\lim_{M\to\infty} \quad \lim_{\Delta\tau\to 0}$$

$$S[X] = \int_0^\beta d\tau \left[\frac{1}{2} m \left(\dot{X}(\tau) \right)^2 + V(X(\tau)) \right]$$ Action



$$Z = \int_{X(0)=X(\beta)} \mathcal{D}X(\tau) e^{-S[X]}$$

Partition function as path integral

Holstein Model: path integral

$$Z = \int \Pi_i \mathcal{D}X_i(\tau)\Pi_{i,\sigma}\mathcal{D}\overline{c}_{i,\sigma}(\tau)\mathcal{D}c_{i,\sigma}(\tau)e^{-S[c,\overline{c},X]}$$

$$S[c,\overline{c},X] = \underbrace{\frac{1}{2}\sum_i \int_0^\beta d\tau \left(\frac{1}{\omega_0^2}\dot{X_i}^2(\tau) + X_i^2(\tau)\right) -}_{S_b}$$

$$\underbrace{-\sum_{i,j,\sigma}\int_0^\beta d\tau \overline{c}_{i,\sigma}(\tau)(\partial_\tau \delta_{i,j} + t_{i,j})c_{j,\sigma}(\tau) + \sqrt{\lambda}\sum_{i,\sigma}\int_0^\beta d\tau X_i(\tau) n_{i,\sigma}(\tau)}_{S_{el}}$$

integrating bosons out...

- Effective fermionic action
- Electron properties

integrating electrons out...

- Effective bosonic action
- Boson properties

Holstein Model: path integral

$$Z = \int \Pi_i \mathcal{D}X_i(\tau)\Pi_{i,\sigma}\mathcal{D}\bar{c}_{i,\sigma}(\tau)\mathcal{D}c_{i,\sigma}(\tau)e^{-S[c,\bar{c},X]}$$

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Holstein Model: integrating electrons out

integrating electrons out...

$$Z = \int \Pi_i \mathcal{D}X_i(\tau) e^{-S_b[X]} \int \Pi_{i,\sigma} \mathcal{D}\bar{c}_{i,\sigma}(\tau) \mathcal{D}c_{i,\sigma}(\tau) e^{-S_{el}[c,\bar{c},X]}$$

$$Z = \int \Pi_i \mathcal{D}X_i(\tau) e^{-S_b[X] - S_{int}[X]}$$

Polarization distribution at site k

$$P(X) = \frac{1}{Z} \int \Pi_i \mathcal{D}X_i(\tau) e^{-S_{ph}[X] - S_{int}[X]} \delta(X - X_k(0))$$

Holstein Model: classical limit

$$S_{ph}[X] = \frac{1}{2}\sum_i \int_0^\beta d\tau \left(\frac{1}{\omega_0^2}\dot{X}_i^{\,2}(\tau) + X_i^2(\tau)\right)$$

$$\omega_0 \to 0$$

$$\dot{X}(\tau) = 0$$
$$X(\tau) = X(0) = X(\beta)$$

$$S_{ph}(X) = \frac{1}{2}\sum_i \beta X_i^2$$

Holstein Model: classical limit

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$$X(\tau) = X(0) = X(\beta)$$

$$S_{ph}(X) = \frac{1}{2}\sum_i \beta X_i^2$$

$$Z = \int \Pi_i dX_i e^{-S_{ph}(X) - S_{int}(X)}$$

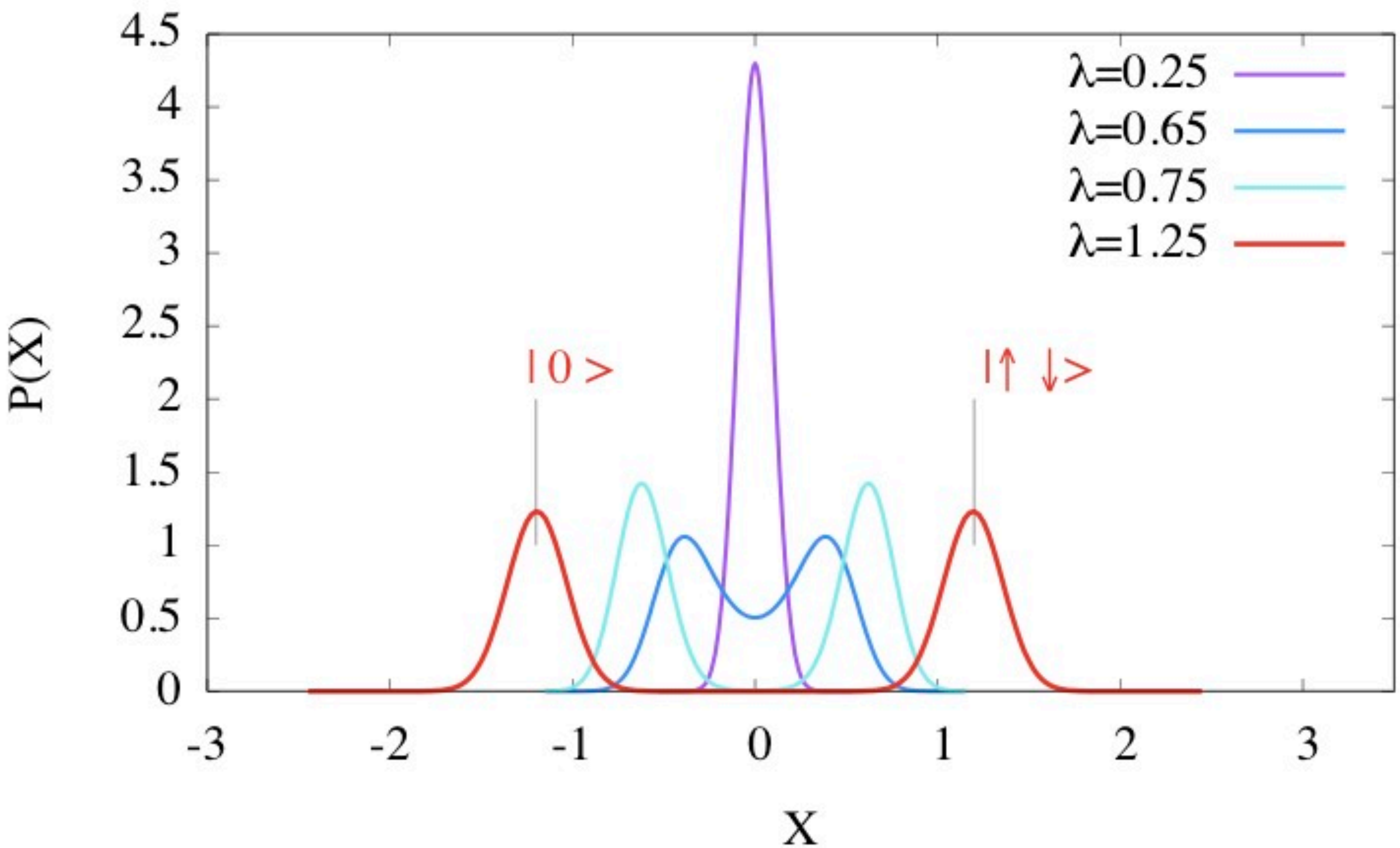
$$S_{int}(X) = -\log\left[\text{tr } e^{-\beta H_{el}(X)}\right]$$

- Classical anharmonic oscillators
- Electrons moving in site-dependent gaussian random potential

Holstein Model: bipolaron formation (DMFT) classical limit

Polarization distribution at impurity site

$$P(X) = \frac{1}{Z}\int dX_0 e^{-S_{ph}(X_0)-S_{int}(X_0)}\delta(X-X_0) \qquad e^{-S_{int}(X_0)} \propto \left(\Pi_n G_0^{-1}(i\omega_n)+gX_0\right)^2$$



[A.J. Millis, Mueller, Shraiman Phys. Rev. B (1996)]
[S.C.,F. de Pasquale Phys. Rev. B (1999)]

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Holstein Model: path integral

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Holstein Model: integrating bosons out

integrating bosons out...

$$Z = \int \Pi_{i,\sigma} \mathcal{D}\bar{c}_{i,\sigma}(\tau)\mathcal{D}c_{i,\sigma}(\tau) \int \Pi_i \mathcal{D}X_i(\tau) e^{-S_{ph}[X] - S_{el}[c,\bar{c},X]}$$

$$Z = \int \Pi_{i,\sigma} \mathcal{D}\bar{c}_{i,\sigma}(\tau)\mathcal{D}c_{i,\sigma}(\tau) e^{-S_{eff}[c,\bar{c}]}$$

$$S_{eff}[c,\bar{c}] = -\sum_{i,j,\sigma}\int_0^\beta d\tau \bar{c}_{i,\sigma}(\tau)(\partial_\tau \delta_{i,j} + t_{i,j})c_{j,\sigma}(\tau) + \frac{\lambda}{2}\sum_{i,\sigma,\sigma'}\int_0^\beta d\tau d\tau' D(\tau-\tau') n_{i,\sigma}(\tau) n_{i,\sigma'}(\tau')$$

$$D(\tau) = -\langle T_\tau X(\tau) X(0)\rangle$$

$$D(i\omega_n) = -\frac{\omega_0^2}{\omega_n^2 + \omega_0^2}$$

Holstein Model: integrating bosons out

integrating bosons out...

$$Z = \int \Pi_{i,\sigma} \mathcal{D}\overline{c}_{i,\sigma}(\tau) \mathcal{D}c_{i,\sigma}(\tau) \int \Pi_i \mathcal{D}X_i(\tau) e^{-S_{ph}[X] - S_{el}[c,\overline{c},X]}$$

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attractive retarded density-density interaction

Holstein Model: large frequency limit

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attractive retarded density-density interaction

$$\omega_0 \to \infty$$

attractive instantaneous density-density interaction

$$S_{eff}[c,\bar{c}] = -\sum_{i,j,\sigma}\int_0^\beta d\tau \bar{c}_{i,\sigma}(\tau)(\partial_\tau \delta_{i,j} + t_{i,j})c_{j,\sigma}(\tau) - \frac{\lambda}{2}\sum_{i,\sigma,\sigma'}\int_0^\beta d\tau n_{i,\sigma}(\tau)n_{i,\sigma'}(\tau)$$

...negative U Hubbard model

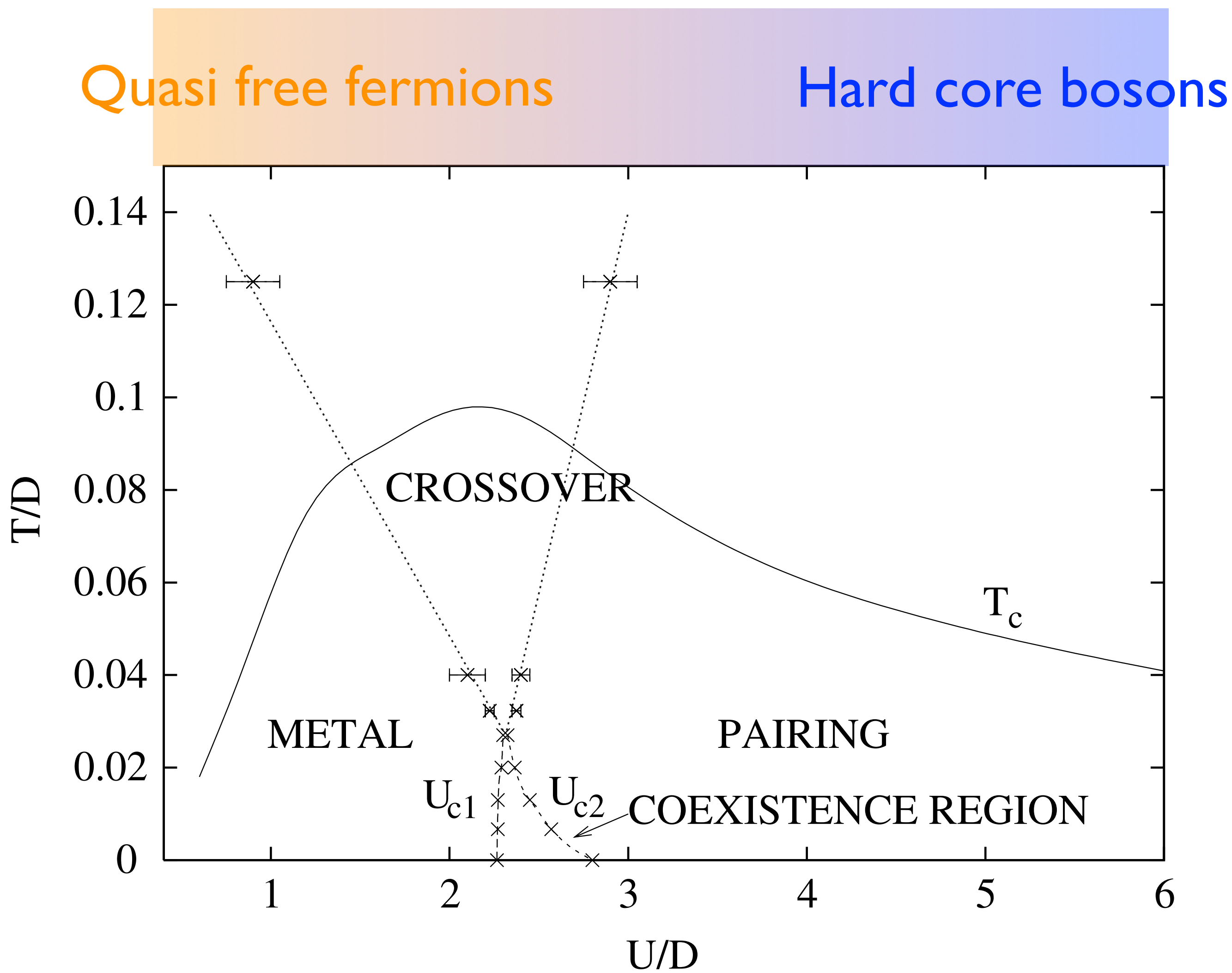
Negative-U Hubbard model

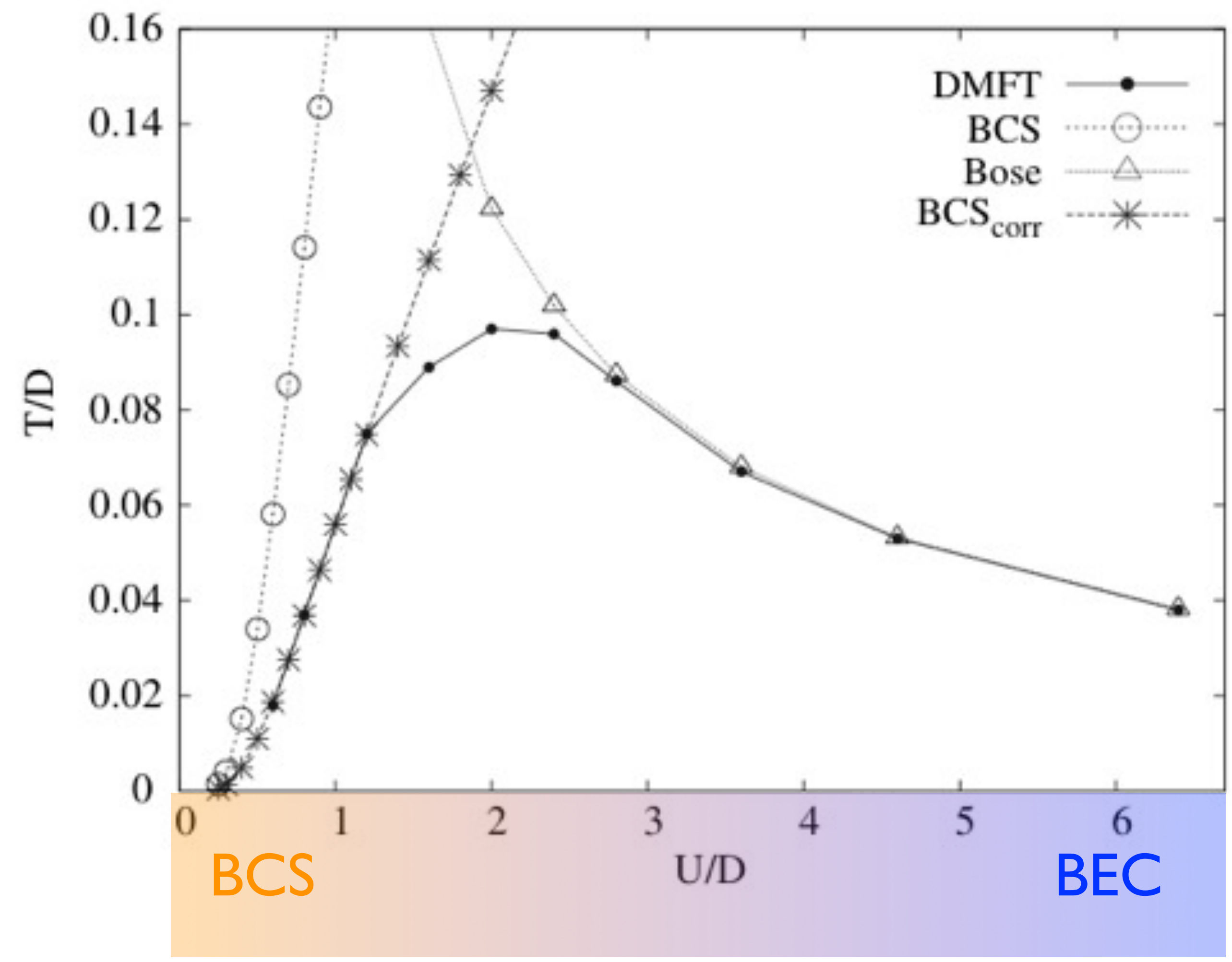
$$H = -t \sum_{<i,j>,\sigma} c^{+}_{i,\sigma} c_{j,\sigma} - U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

attractive coupling: $U = \dfrac{2g^2}{\omega_0}$ (bipolaron binding energy)

adimensional e-e coupling: $\dfrac{U}{D} = \lambda$

Negative-U Hubbard model: DMFT phase diagram at half filling





[A. Toschi, P. Barone, M. Capone C. Castellani NJP 7, 7 (2005)]

Holstein Model: large frequency limit

restoring the “boson” variables...

$$S[c,\bar{c},X] = \frac{1}{2}\sum_i \int_0^\beta d\tau \left(\cancel{\frac{1}{\omega_0^2}\dot{X}_i^2(\tau)} + X_i^2(\tau) \right) -$$

$$- \sum_{i,j,\sigma} \int_0^\beta d\tau \bar{c}_{i,\sigma}(\tau)(\partial_\tau \delta_{i,j} + t_{i,j}) c_{j,\sigma}(\tau) + \sqrt{\lambda} \sum_{i,\sigma} \int_0^\beta d\tau X_i(\tau) n_{i,\sigma}(\tau)$$

“bosons” becomes Hubbard-Statonvich variables...

$$\exp(\frac{1}{2}\hat{A}^2) = \frac{1}{\sqrt{2\pi}} \int dx \exp(-\frac{1}{2}x^2 + x\hat{A})$$

- H-S variables conjugated to density (attraction)
- H-S variables have no defined polarization

$$X = \sqrt{\frac{\omega_0}{2}}(a + a^\dagger)$$

$$< X^2 > \rightarrow \infty$$

Holstein Model: large frequency limit

restoring the “boson” variables...

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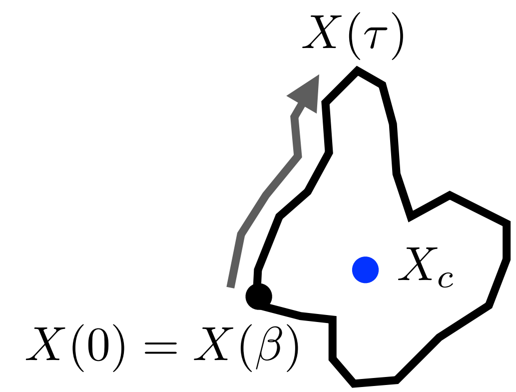
Can we describe pairing by means distribution functions of H-S variables?

Path integrals: end-point & centroid



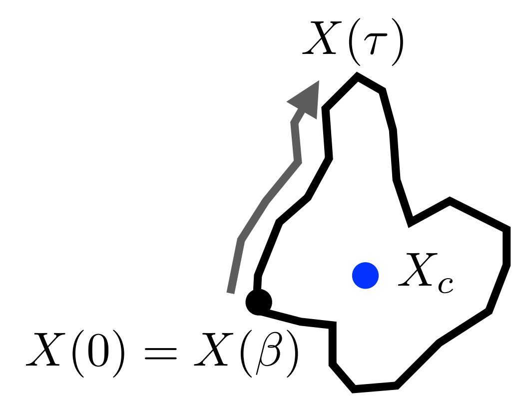
endpoint

$$X(0) = X(\beta)$$

centroid:"classical" position of the quantum particle

$$X_c = \frac{1}{\beta}\int_0^\beta d\tau X(\tau)$$

End-point & centroid for an harmonic oscillator



endpoint distribution → thermal+quantum fluctuations

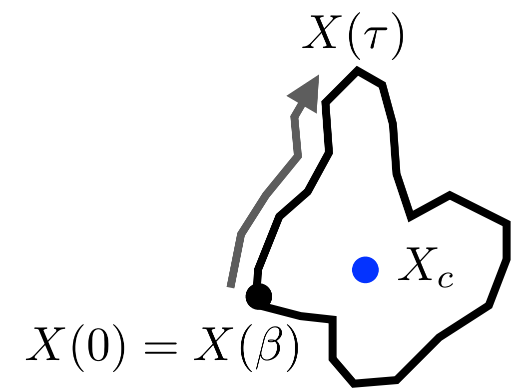
$$P(X) \propto \exp(-\frac{X^2}{\xi^2(T)}) \qquad \xi^2(T) = \frac{\hbar\omega_0}{k \tanh(\beta\hbar\omega_0/2)}$$

centroid distribution → thermal fluctuations

$$P(X_c) \propto \exp(-\frac{X_c^2}{2\xi_c^2(T)}). \qquad \xi_c^2(T) = \frac{k}{\beta}$$

centroid distribution is non-trivial for H-S variables ($\hbar\omega_0 \to \infty$)

Path integrals: end-point & centroid



endpoint

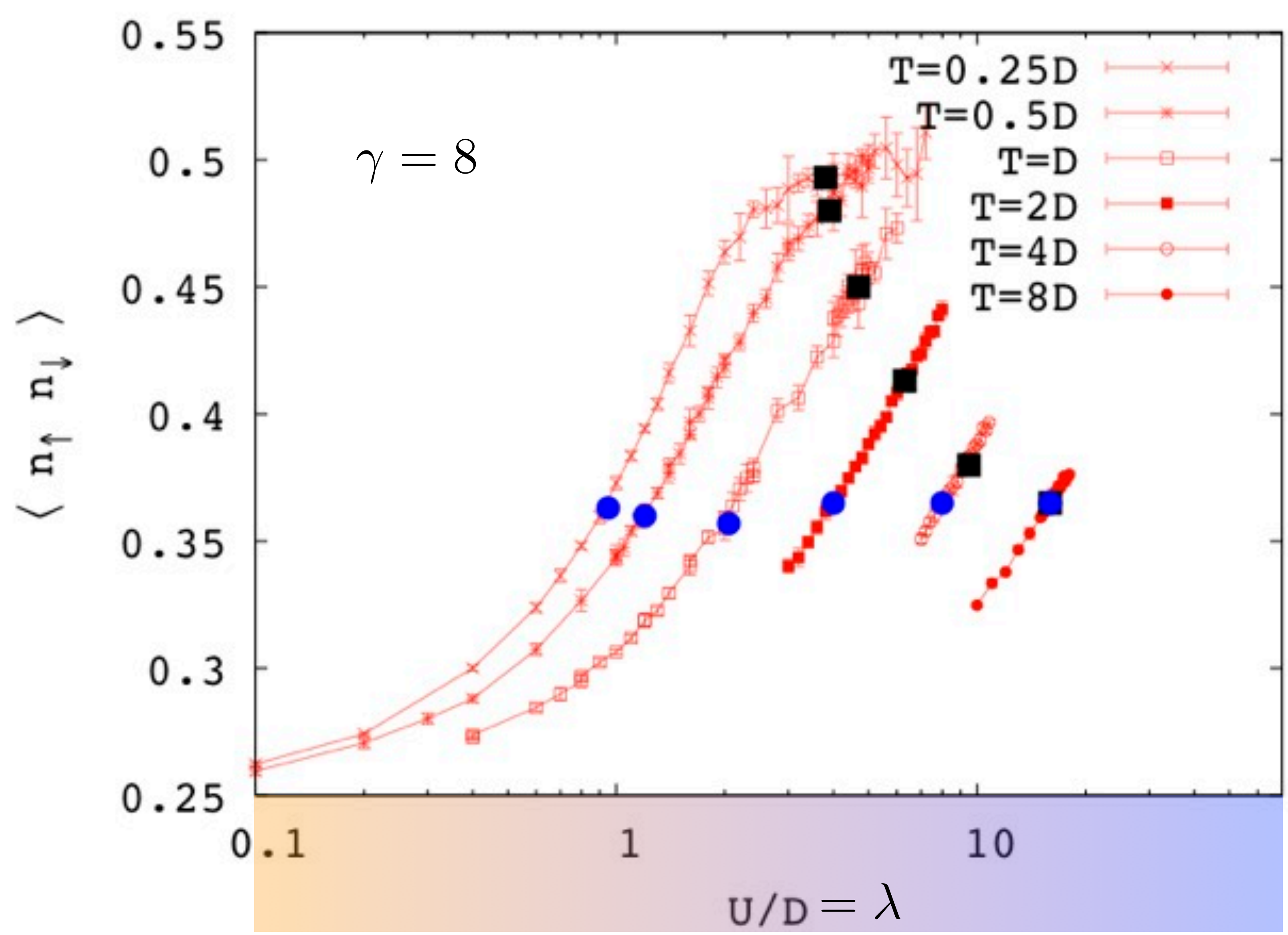
$$X(0) = X(\beta) \longrightarrow$$ bimodality of P(X): polarization crossover

centroid

$$X_c = \frac{1}{\beta}\int_0^\beta d\tau X(\tau) \longrightarrow$$ bimodality of P(X_c): paring crossover

Holstein model: pairing (DMFT)

centroid distribution bimodality → location of the pairing crossover



[S. C., G. Sangiovanni, and M. Capone Phys. Rev. B 73, 245114 (2006)]

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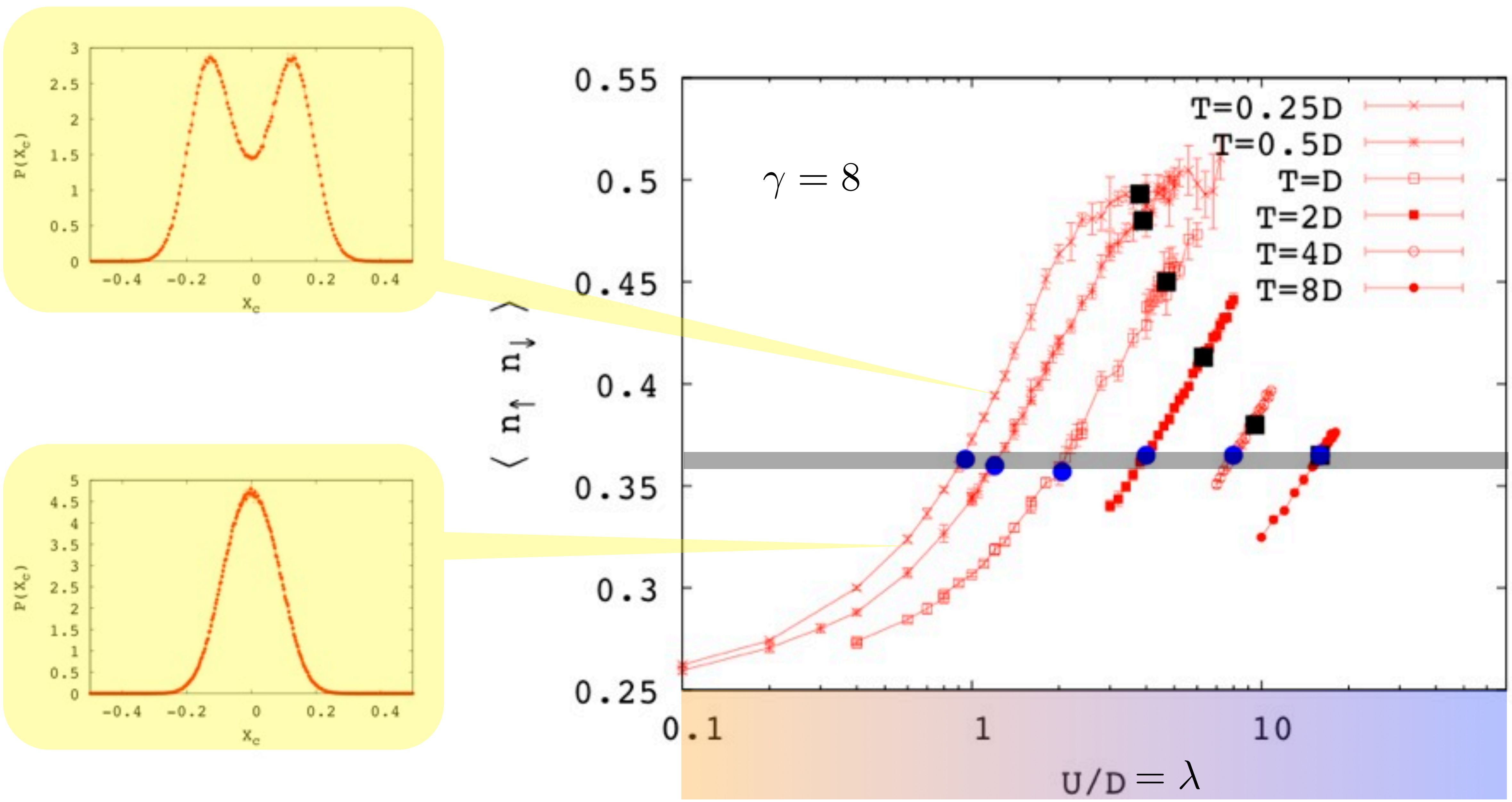
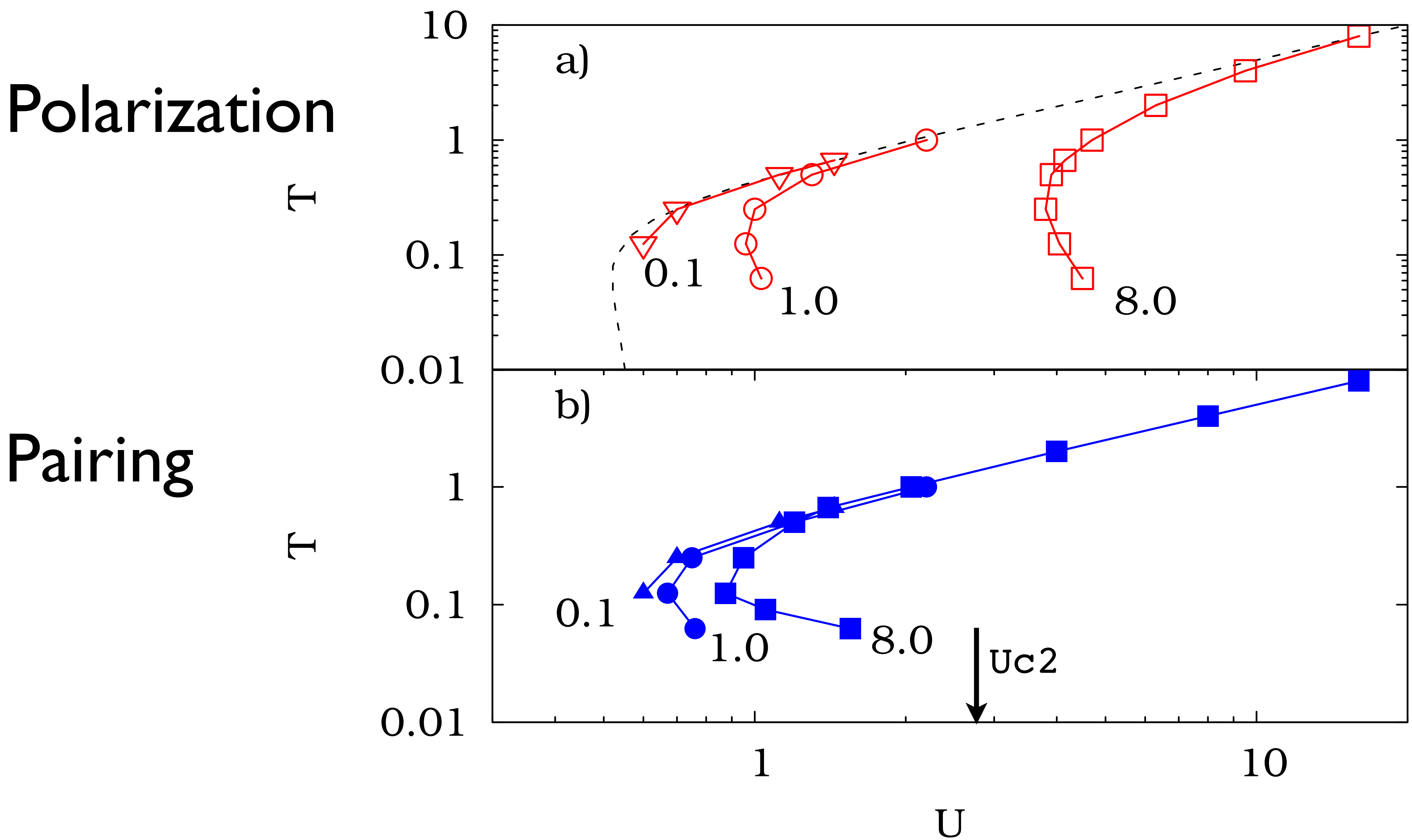


[S. C., G. Sangiovanni, and M. Capone Phys. Rev. B 73, 245114 (2006)]

Holstein model: DMFT phase diagram at half-filling



[S. C., G. Sangiovanni, and M. Capone Phys. Rev. B 73, 245114 (2006)]

The "classical" FDT for centroids

Fluctuations-Response

Static external field h_i coupled locally with an operator $\hat{m}_i$

$$H = H' - \sum_i h_i \hat{m}_i$$

Static response

$$\chi_{i,j} = \frac{\delta}{\delta h_j} < \hat{m}_i > \Big|_{h=0}$$

$$\chi_{i,j} = \int_0^\beta d\tau \, [< \hat{m}_i(\tau) \hat{m}_j(0) > - < \hat{m}_i(\tau) >< \hat{m}_j(0) >]_{h=0}$$

Classical limit ($\beta \to 0$)

$$\chi_{i,j} = \beta \, [< \hat{m}_i \, \hat{m}_j > - < \hat{m}_i >< \hat{m}_j >]_{h=0}$$

The “classical” FDT for centroids

Fluctuations-Response

Static external field h_i coupled locally with an operator $\hat{m}_i$

$$H = H' - \sum_i h_i \hat{m}_i$$

Quadratic interaction...

$$H' = H_0 - \frac{U}{2} \sum_i \hat{m}_i^2$$

...linearized by H-S transformation

$$S'[X] = S_0 + \frac{1}{2} \sum_i \int d\tau X_i^2(\tau) - \sqrt{U} \sum_i \int d\tau X_i(\tau) m_i(\tau)$$

“classical” fluctuations-response for centroids

$$\chi_{i,j} = \frac{1}{U} \left[\beta (< X_{c,i} X_{c,j} > - < X_{c,i} >< X_{c,j} >) - \delta_{i,j} \right]$$

The “classical” FDT for centroids

“classical” fluctuations-response for centroids

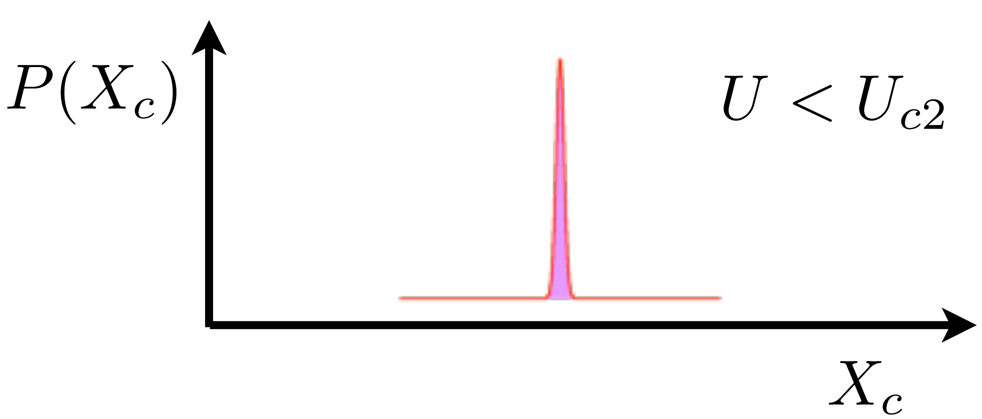
$$\chi_{i,j} = \frac{1}{U}\left[\beta(< X_{c,i}X_{c,j} > - < X_{c,i} >< X_{c,j} >) - \delta_{i,j}\right]$$

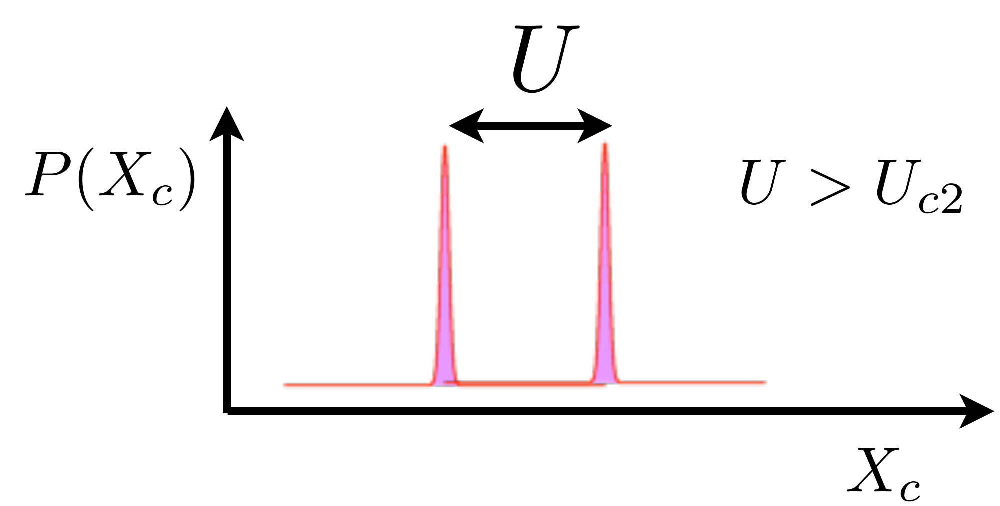
Half-filled negative-U Hubbard model (DMFT) ($\beta \to \infty$) (*)

$$U < U_{c2} \qquad \chi^c_{i,i} \simeq \frac{k}{1 - U/U_{c2}} \qquad \Longrightarrow \qquad < \Delta X_c^2 > \simeq \frac{U}{\beta}\frac{k}{1 - U/U_{c2}}$$

$$U > U_{c2} \qquad \chi^c_{i,i} \simeq \beta \qquad\qquad < \Delta X_c^2 > \simeq U$$

Centroid distribution across MIT





[(*) A. Georges et al. Rev. Mod. Phys. 68, 13–125 (1996)]

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Negative vs positive U at half-filling

Negative U

$$H = H_0 - \frac{U}{2}\sum_i (n_{i,\uparrow} + n_{i,\downarrow} - 1)^2$$

$$\rho_{i,z} = n_{i,\uparrow} + n_{i,\downarrow} - 1$$

$$\boldsymbol{\rho} = (c^\dagger_\uparrow, c_\downarrow)\, \boldsymbol{\sigma} \begin{pmatrix} c_\uparrow \\ c^\dagger_\downarrow \end{pmatrix}$$

Positive U

$$H = H_0 - \frac{U}{2}\sum_i (n_{i,\uparrow} - n_{i,\downarrow})^2$$

$$m_{i,z} = n_{i,\uparrow} - n_{i,\downarrow}$$

$$\mathbf{m} = (c^\dagger_\uparrow, c^\dagger_\downarrow)\, \boldsymbol{\sigma} \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$$

Negative vs positive U at half-filling

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- H-S variable conjugated to pseudo-spin
- Bimodality of charge centroid distribution → local pairs
- Centroid variance → local charge susceptibility

Positive U

$$H = H_0 - \frac{U}{2}\sum_i (n_{i,\uparrow} - n_{i,\downarrow})^2$$

$$m_{i,z} = n_{i,\uparrow} - n_{i,\downarrow}$$

$$\mathbf{m} = (c_\uparrow^\dagger, c_\downarrow^\dagger)\,\boldsymbol{\sigma}\begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$$

- H-S variable conjugated to spin
- Bimodality of spin centroid distribution → local moments
- Centroid variance → local spin susceptibility

Negative vs positive U at half-filling

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$$\mathbf{m} = (c_\uparrow^\dagger, c_\downarrow^\dagger)\,\boldsymbol{\sigma}\begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$$

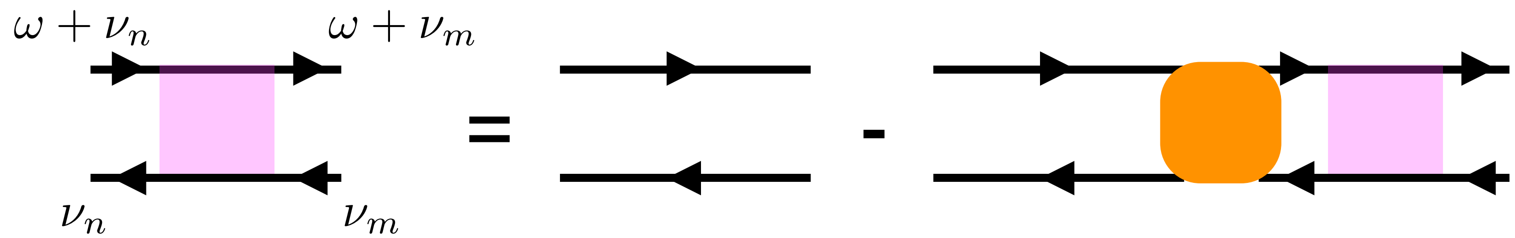
Use the bimodality of charge centroid distribution in the Holstein model at large frequency to guess the position of the Fermi liquid / local moments crossover in the positive U Hubbard model (DMFT)

Compare the position of this crossover with that of precursor of the Mott transition (DMFT)

Divergent precursor of the Mott transition

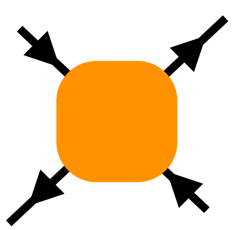
local charge susceptibility matrix (DMFT)

$$[\boldsymbol{\chi}(\omega)]_{n,m} = \int d\tau_1 d\tau_2 d\tau_3 e^{-i\nu_n \tau_1} e^{(\nu_n+\omega)\tau_2} e^{-i(\nu_m+\omega)\tau_3} \times$$
$$\times \left\langle T_\tau c^\dagger(\tau_1) c(\tau_2) c^\dagger(\tau_3) c(0) \right\rangle - \left\langle T_\tau c^\dagger(\tau_1) c(\tau_2) \right\rangle \left\langle T_\tau c^\dagger(\tau_3) c(0) \right\rangle$$



$$\boldsymbol{\chi} = \boldsymbol{\chi}_0 - \boldsymbol{\chi}_0 \boldsymbol{\Gamma} \boldsymbol{\chi}$$

Bethe-Salpeter equation



$$\boldsymbol{\Gamma} = \boldsymbol{\chi}^{-1} - \boldsymbol{\chi}_0^{-1}$$

irreducible (p-h) vertex

[T. Schäfer, G. Rohringer,O. Gunnarsson, S. C., G. Sangiovanni, and A. Toschi PRL 110, 246405 (2013)]

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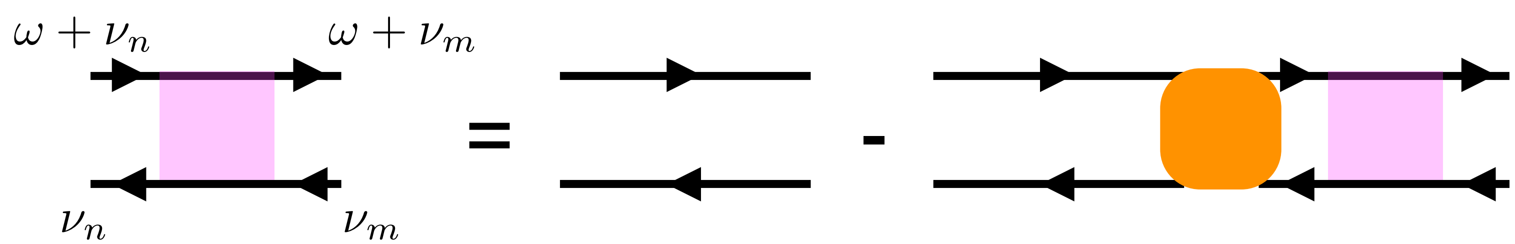
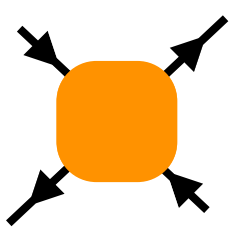
$$\times \left\langle T_\tau c^\dagger(\tau_1)c(\tau_2)c^\dagger(\tau_3)c(0)\right\rangle - \left\langle T_\tau c^\dagger(\tau_1)c(\tau_2)\right\rangle \left\langle T_\tau c^\dagger(\tau_3)c(0)\right\rangle$$



$$\boldsymbol{\chi} = \boldsymbol{\chi}_0 - \boldsymbol{\chi}_0 \boldsymbol{\Gamma} \boldsymbol{\chi}$$

Bethe-Salpeter equation



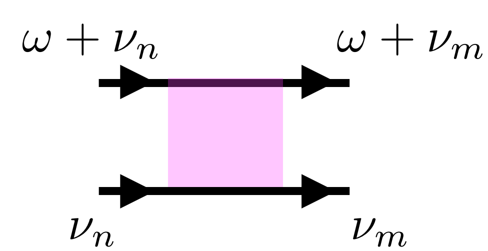
$$\boldsymbol{\Gamma} = \boldsymbol{\chi}^{-1} - \boldsymbol{\chi}_0^{-1}$$

irreducible (p-h) vertex

charge $\qquad \boldsymbol{\chi}_c = \boldsymbol{\chi}_{\uparrow\uparrow} + \boldsymbol{\chi}_{\uparrow\downarrow}$

p-p $\qquad \boldsymbol{\chi}_{pp}$

spin $\qquad \boldsymbol{\chi}_s = \boldsymbol{\chi}_{\uparrow\uparrow} - \boldsymbol{\chi}_{\uparrow\downarrow}$



Divergent precursor of the Mott transition

Γ charge: diverges at $\omega=\nu n=\nu m=0$ at $T_{p\text{-}h}(U)$

Γ p-p: diverges at $\omega=\nu n=\nu m=0$ at $T_{p\text{-}p}(U)$

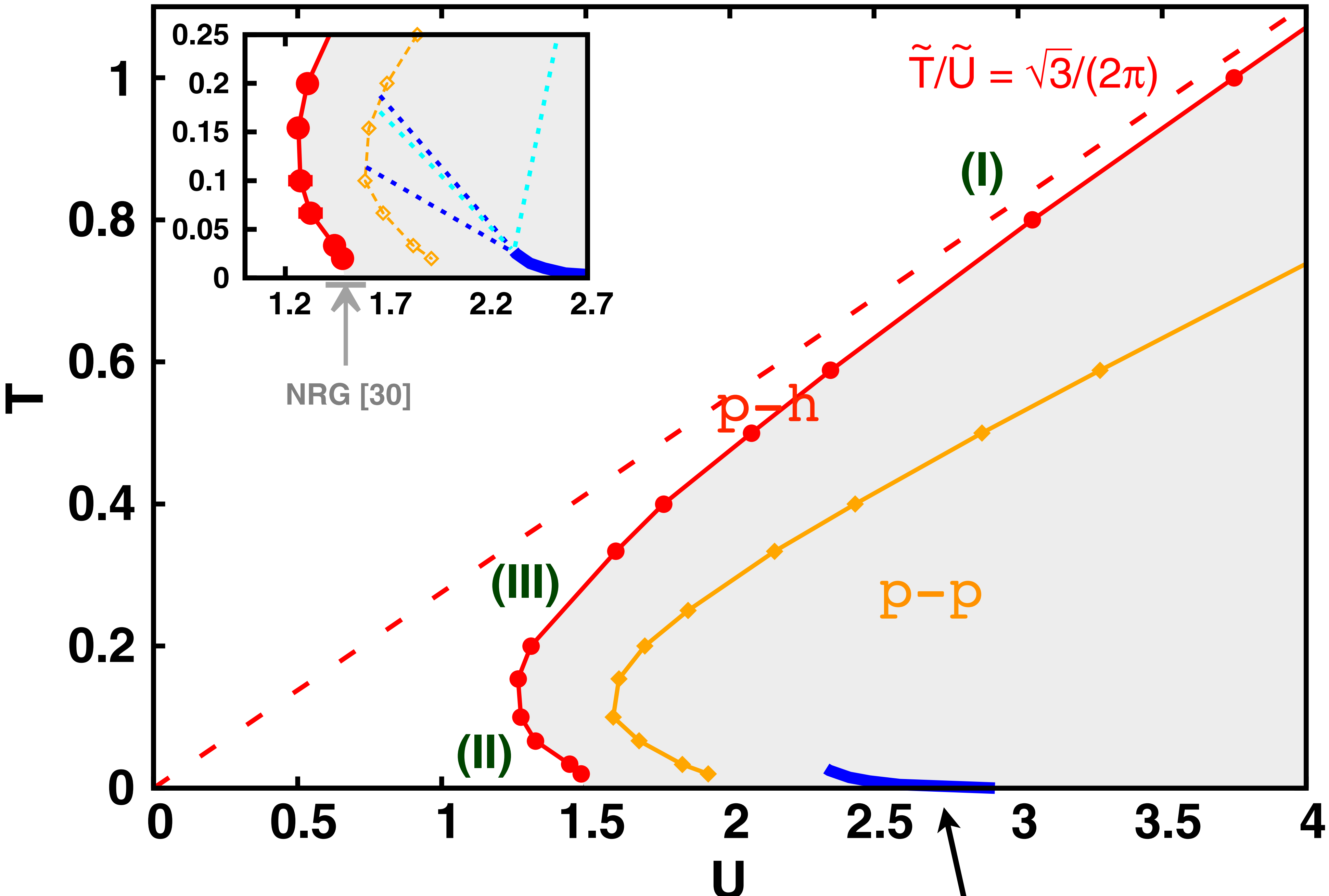
Γ spin: regular

Divergence of Γ imply beaking of Kadanoff-Baym perturbation theory

$$\frac{\delta\Phi[G]}{\delta G(1,2)} = \Sigma(1,2)$$

$$\frac{\delta^2\Phi[G]}{\delta G(3,4)\delta G(1,2)} = \Gamma(1,2,3,4)$$

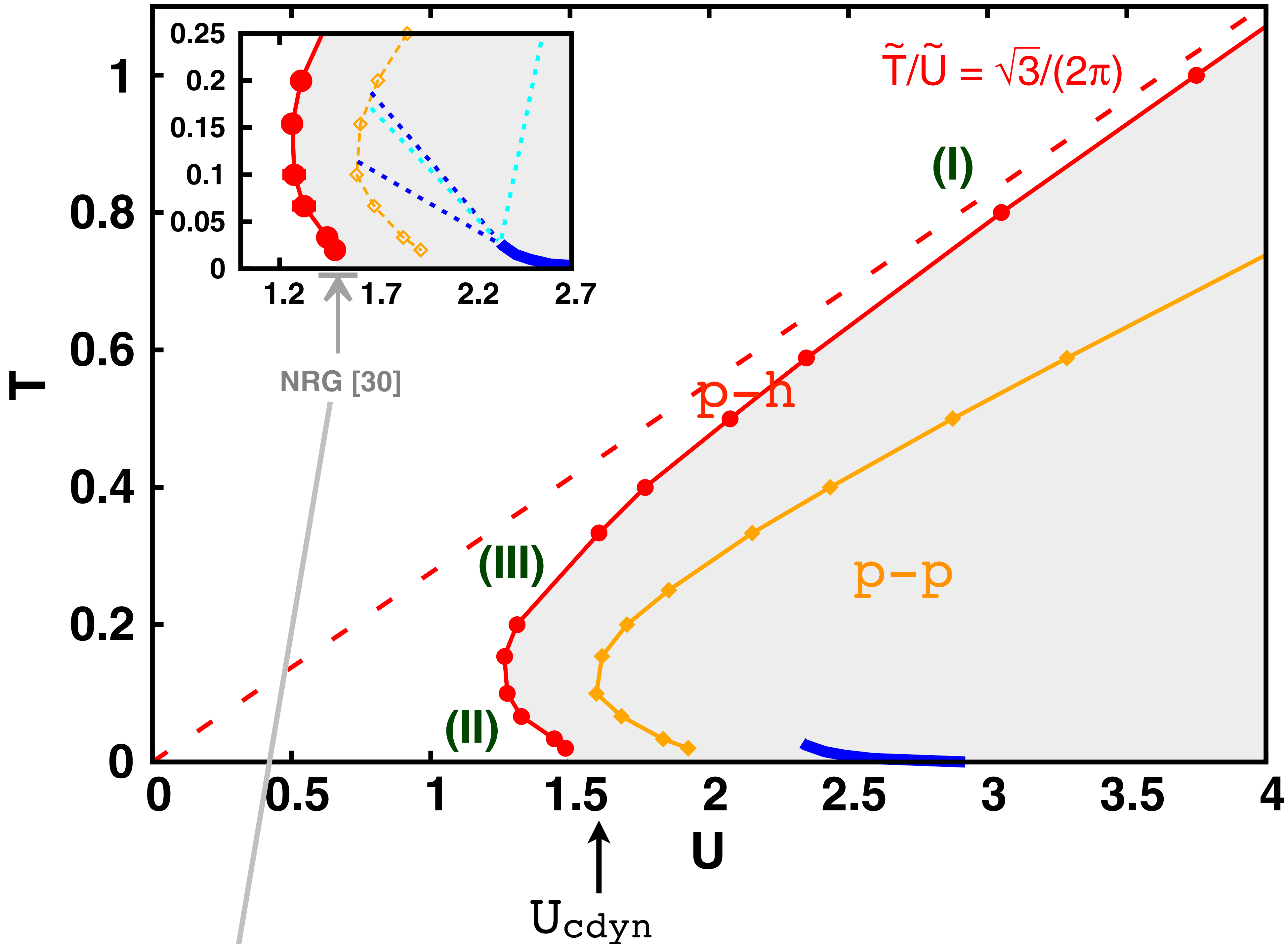
Divergent precursor of the Mott transition



[N.Blumer, Ph.D thesis, Augsburg, (2003)]

[T. Schäfer, G. Rohringer, O. Gunnarsson, S. C., G. Sangiovanni, and A. Toschi PRL 110, 246405 (2013)]

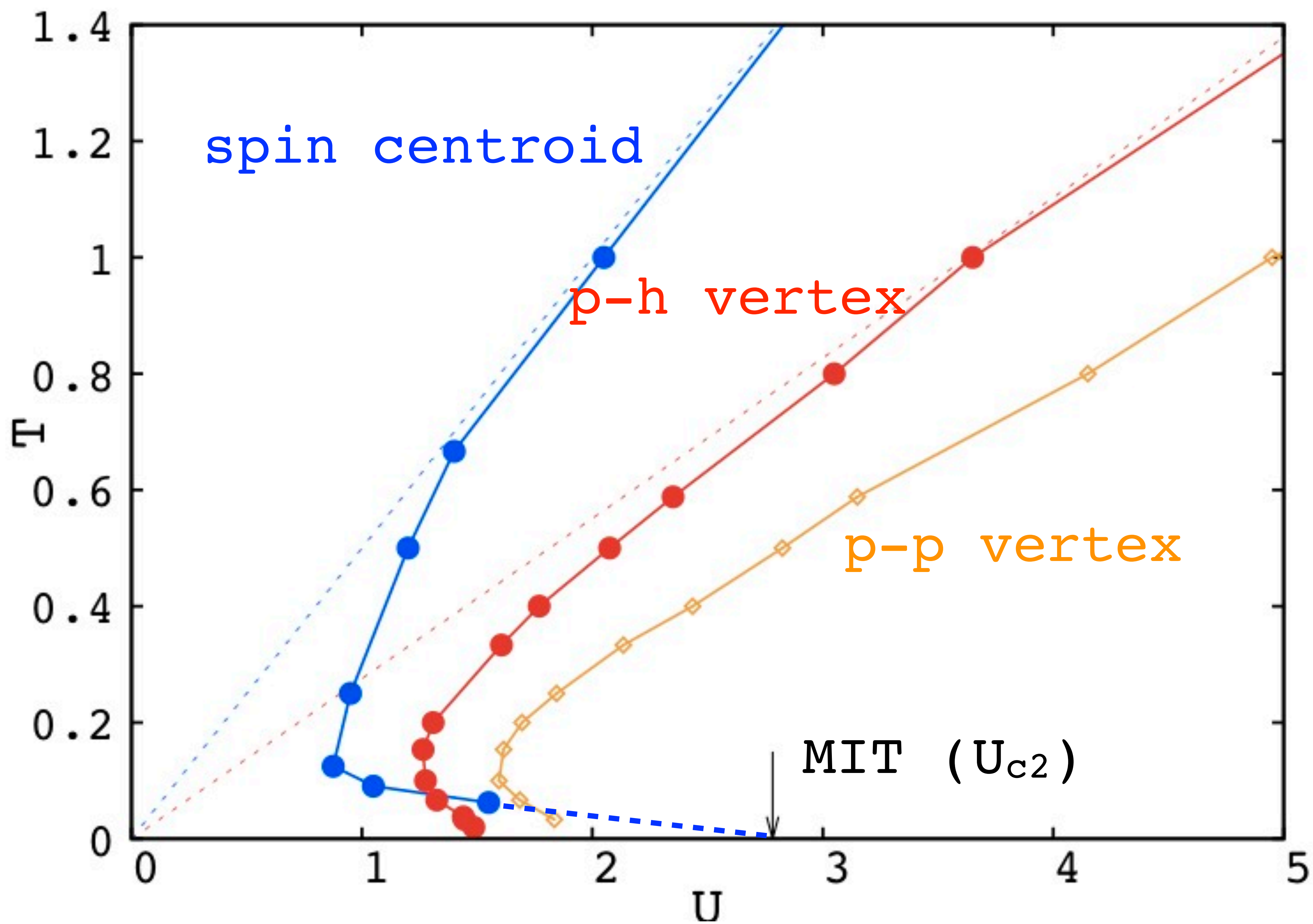
Divergent precursor of the Mott transition



[M.Eckstein, M.Kollar,P.Werner PRL 103, 056403 (2009)]

[R. Zitzler, Ph.D. thesis, Augsburg, (2004); R. Bulla PRL 83, 136 (1999)

Vertex divergence and centroid bimodality



[T. Schäfer, G. Rohringer,O. Gunnarsson, S. C., G. Sangiovanni, and A. Toschi PRL 110, 246405 (2013)]

Generalized centroid distributions

arbitrariness in choosing H-S decoupling

$$H = H_0 - \frac{U}{2}\sum_i \rho_{i,z}^2 \quad \longrightarrow \quad H = H_0 - \frac{U}{2}\sum_i \rho_{i,n}^2$$

integrate over equivalent directions n

$$\begin{array}{cc} & \begin{array}{cccc} |\uparrow\downarrow> & |0> & |\uparrow> & |\downarrow> \end{array} \\ \rho_n = & \begin{pmatrix} \cos(\theta) & \sin(\theta)e^{-i\phi} & 0 & 0 \\ \sin(\theta)e^{i\phi} & -\cos(\theta) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array}$$

$$Z = \int \Pi_i \mathcal{D}\Omega_i(\tau)\mathcal{D}X_i(\tau)e^{-S_{HS}[X]} \int \Pi_{i,\sigma}\mathcal{D}\overline{c}_{i,\sigma}(\tau)\mathcal{D}c_{i,\sigma}(\tau)e^{-S_{el}[c,\overline{c},X,\theta,\phi]}$$

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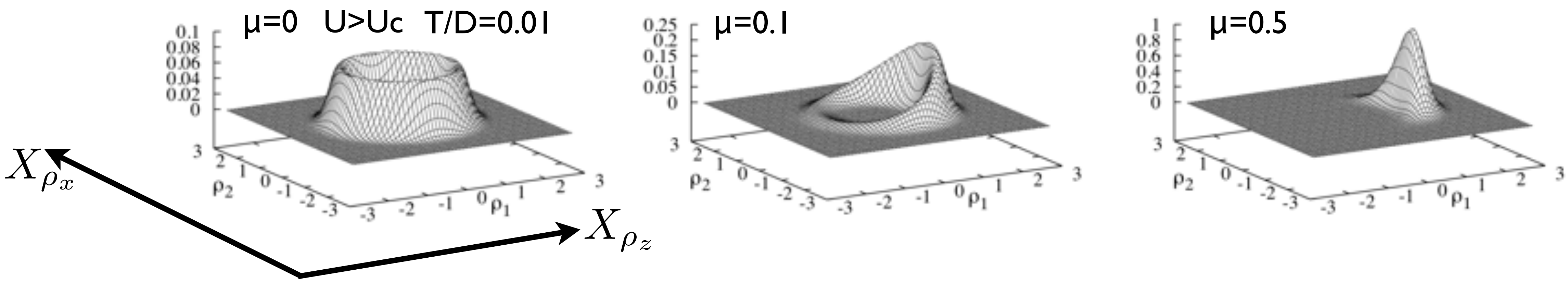
$$Z = \int \Pi_i \mathcal{D}\Omega_i(\tau)\mathcal{D}X_i(\tau)e^{-S_{HS}[X]-S_{int}[X,\theta,\phi]}$$

generalized centroid distributions

$$X_{\rho_x} \Longleftrightarrow \rho_x = c_\uparrow^\dagger c_\downarrow^\dagger + c_\downarrow c_\uparrow$$



[F. de Pasquale S.C. Physica B 284, 1573 (2000)]

Centroid distribution from auxiliary field QMC

QMC for ground state

$$|\Psi_0 >= \lim_{\beta\to\infty} e^{-\beta(H-E_T)}|\Psi_T >= \lim_{M\to\infty} \Pi_{i=1,M} e^{-\Delta\tau(H-E_T)}|\Psi_T >$$

$$e^{-\Delta\tau H} = e^{-\Delta\tau H_0/2} e^{-\Delta\tau V} e^{-\Delta\tau H_0/2} + o(\Delta\tau^2)$$

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Auxiliary fields (H-S transformation)

$$V = -A^2$$

$$\exp(\frac{1}{2}\hat{A}^2) = \frac{1}{\sqrt{2\pi}} \int dx \exp(-\frac{1}{2}x^2 + x\hat{A}) \qquad x_c = \frac{1}{M}\sum_{i=1}^{M} x_i$$

- Distribution of centroids is a byproduct of QMC scheme
- Easy access to response by use of FDT for centroids

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[Hao Shi and Shiwei Zhang arXiv:1307.2147 (2013)]

Charge H-S decoupling can improve stat. errors w.r.t. discrete spin Hirsh-Fye decoupling in the positive U Hubbard model

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Conclusions

❖ Analysis of bosonic path statistics can provide a method to determine the local polarization crossover in the normal state for a polaronic system as well as the pairing crossover once centroids of the bosonic paths are considered.

❖ Using the same method it is possible to locate the spin crossover from Fermi Liquid to Local Spin in the normal phase of the positive U Hubbard models.

❖ A general relation holds between centroid moments and generalized N-particle susceptibilities. In particular a “classical” relation holds between the variance of the centroid and the susceptibility of the conjugated variable.

❖ Centroid distributions are byproduct of Auxiliary Field QMC.

❖ Divergence of the irreducible local vertex (p-p,p-h) is a precursor of the Mott transition at zero temperature but occurs well inside the local spin region at high temperature.

Is there a qualitative difference between the intermediate U low temperature regime T<0.1D and the high temperature regime T>0.1D?

Test the relation between vertex anomaly and non-equilibrium properties in the Falicov-Kimball model (CPA)