Efficient treatment of phonons and frequency dependent interactions in DMFT

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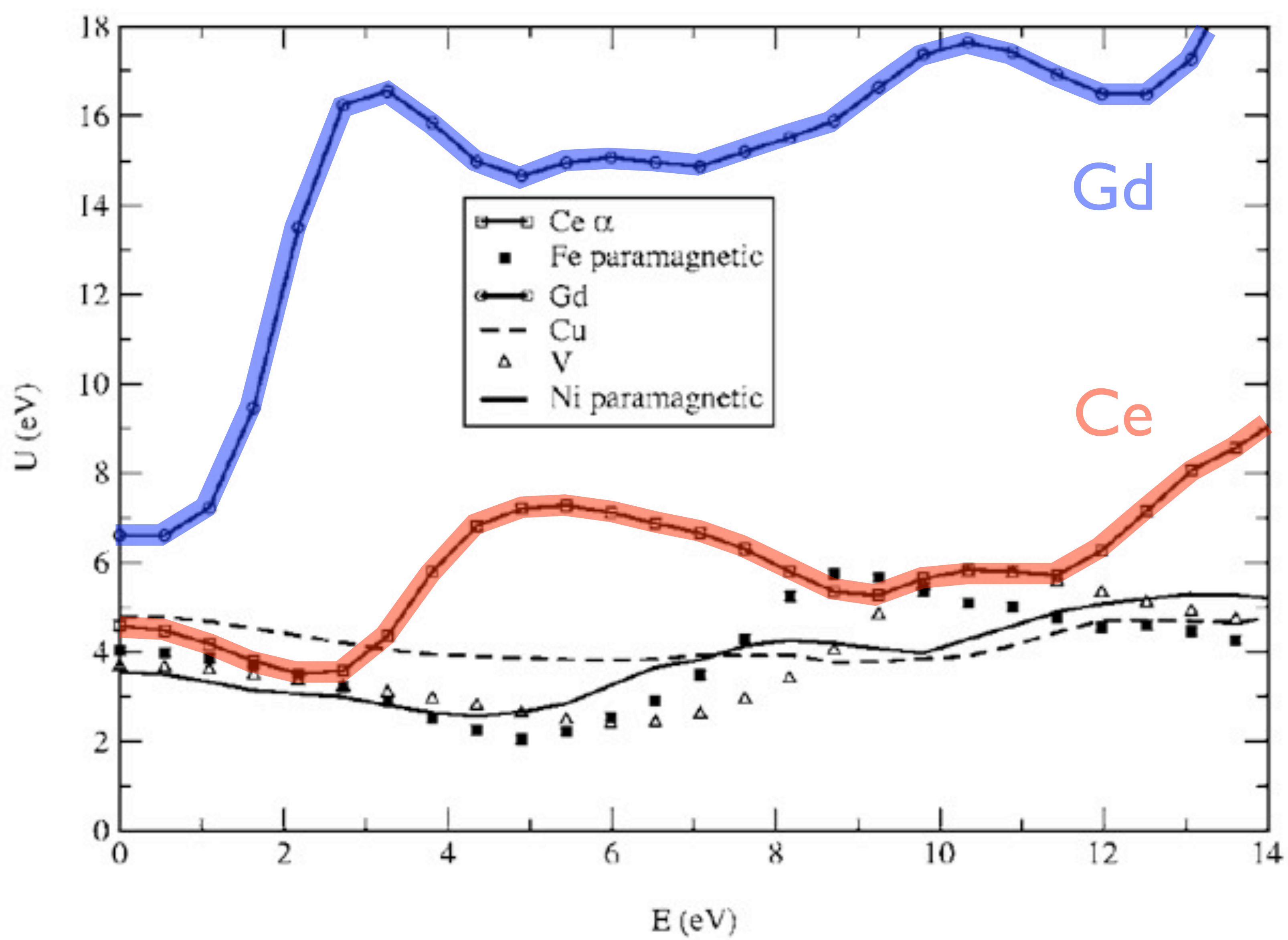
KITP, January 2010

Motivation

Aryasetiawan, Imada, Georges, Kotliar, Biermann & Lichtenstein, PRB (2005)
Aryasetiawan, Karlsson, Jepsen, Schönberger, PRB (2006)
Miyake and Aryasetiawan, PRB (2008)

- Gd, Ce, ... : ab-initio calculation of interaction parameters yields strong frequency dependence



Outline

- Introduction / reminder
  - Hybridization expansion for the Hubbard model
- Electron-phonon coupling
  - Hybridization expansion for the Holstein-Hubbard model
- Frequency-dependent interactions
  - Frequency-dependent U for the Holstein-Hubbard model
  - General formalism
- Application
  - Metal-insulator transition

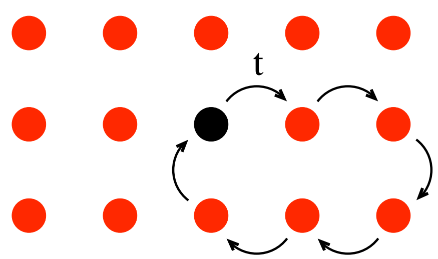
- Collaborators
  - Andy Millis (Columbia)

Dynamical mean field theory

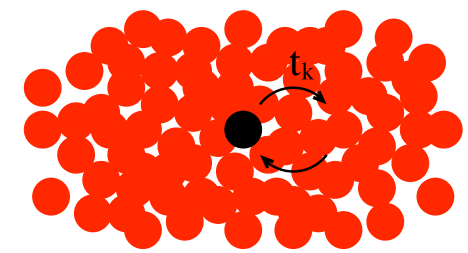
Metzner & Vollhardt, PRL (1989)
Georges & Kotliar, PRB (1992)

- Self-consistency loop

lattice model



impurity model



$$G_{latt} \Longrightarrow H_{imp}$$

$G_{latt} \equiv G_{imp}$

$$\int dk \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{latt}}$$

impurity solver

$$\Sigma_{latt} \Longleftarrow G_{imp},\ \Sigma_{imp}$$

$\Sigma_{latt} \equiv \Sigma_{imp}$

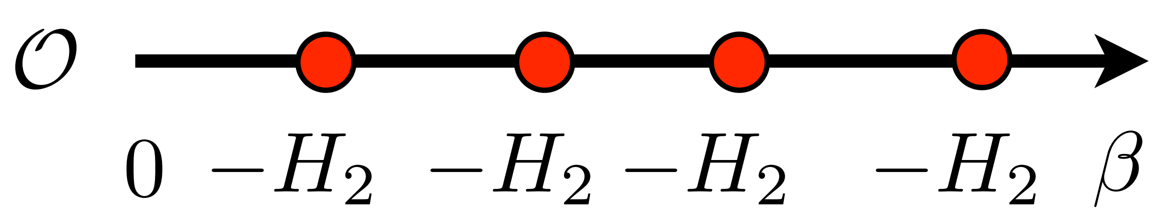
Continuous-time QMC

Rubtsov, Savkin & Lichtenstein, PRB (2005)
Werner et al., PRL (2006)

- Interaction picture

$$H = H_1 + H_2, \quad \mathcal{O}(\tau) = e^{\tau H_1} \mathcal{O} e^{-\tau H_1}$$

$$\langle \mathcal{O} \rangle = \frac{1}{Z} Tr\left[e^{-\beta H} \mathcal{O}\right] = \frac{1}{Z} Tr\left[e^{-\beta H_1} \left(T_\tau e^{-\int_0^\beta d\tau H_2(\tau)}\right) \mathcal{O}\right]$$



Expand time evolution operator in powers of H_2

- Weak-coupling expansion: $H_2 = \text{interaction term}$
- ``Strong-coupling'' expansion: $H_2 = \text{hybridization term}$

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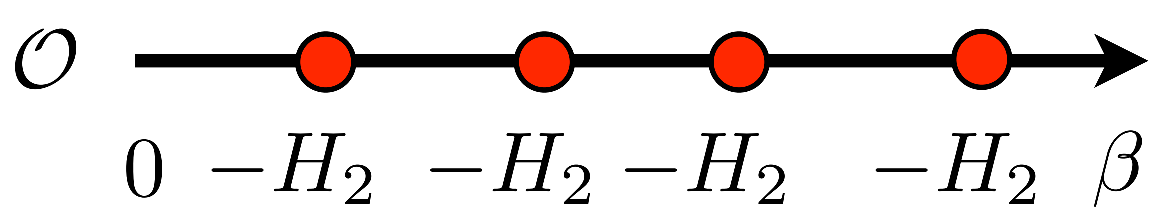

Expand time evolution operator
in powers of H_2

- Sample Monte Carlo configurations through random insertions and removals of (pairs) of operators
- Measure contribution to $\mathcal{O}$

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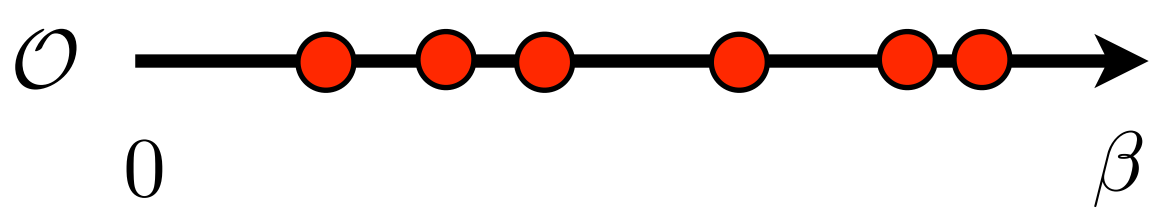

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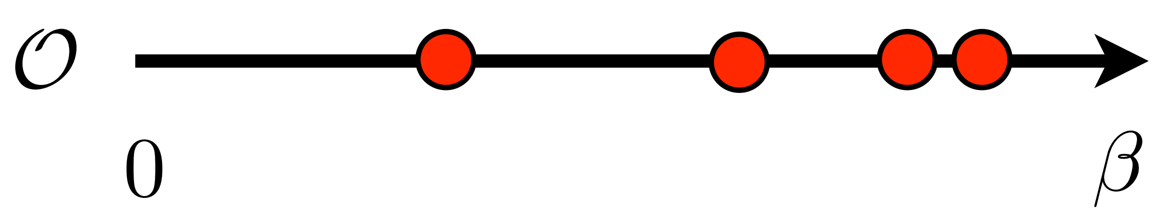

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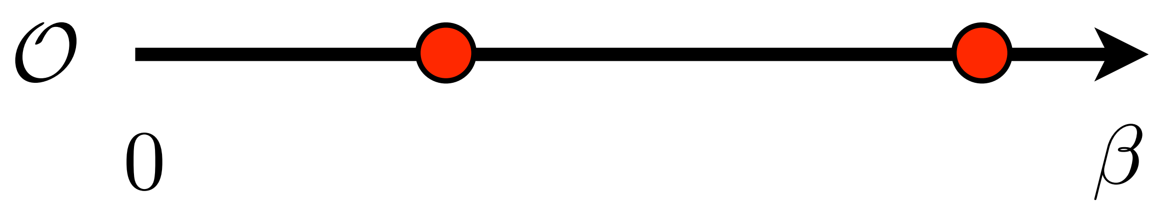

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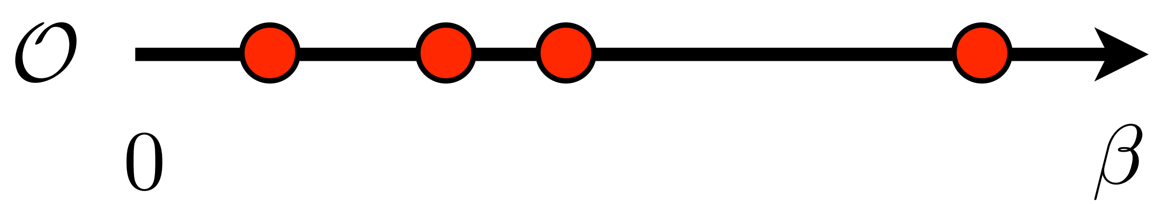

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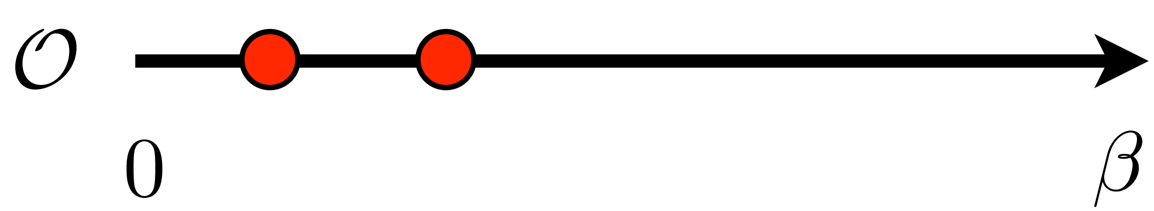

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Hybridization expansion

Werner et al., PRL (2006)

- Hybridization expansion for the Hubbard model

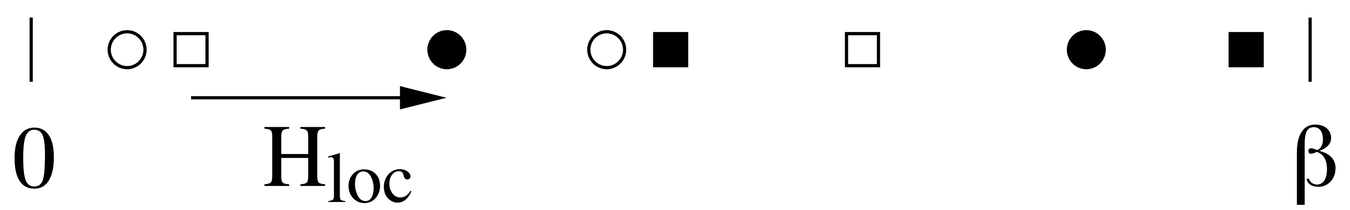
$$
\begin{aligned}
H &= \underbrace{H_{\mathrm{loc}} + H_{\mathrm{bath}}}_{H_1} + \underbrace{H_{\mathrm{hyb}}}_{H_2} \\
H_{\mathrm{loc}} &= -\mu(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow \\
H_{\mathrm{bath}} &= \sum_{p\sigma} \epsilon_p a^\dagger_{p\sigma} a_{p\sigma} \\
H_{\mathrm{hyb}} &= \sum_{p\sigma} V_{p\sigma} c^\dagger_\sigma a_{p\sigma} + h.c.
\end{aligned}
$$

- Expand partition function in powers of $H_2 = H_{\mathrm{hyb}}$
- Compute $Tr_c Tr_a[\ldots]$

Hybridization expansion

Werner et al., PRL (2006)

- Monte Carlo configurations consist of *2n* impurity creation and annihilation operators $\{O_i(\tau_i)\}_{0<\tau_1<\ldots<\tau_{2n}}$



$$w_{\text{Hubbard}}(\{O_i(\tau_i)\}) = Tr_c\left[e^{-\beta H_{\text{loc}}} O_{2n}(\tau_{2n}) \ldots O_1(\tau_1)\right] \times d\tau_1 \ldots d\tau_{2n} \det M_\uparrow(V,\epsilon) M_\downarrow(V,\epsilon)$$

- $Tr_a[\ldots]$ yields two determinants of hybridization matrices
- $Tr_c[\ldots]$ must be computed explicitly

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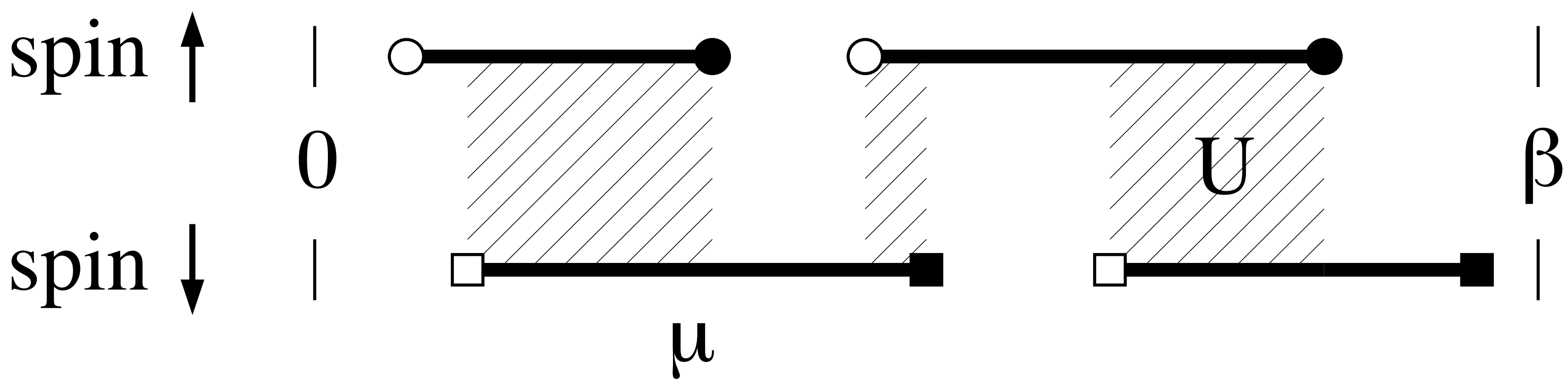

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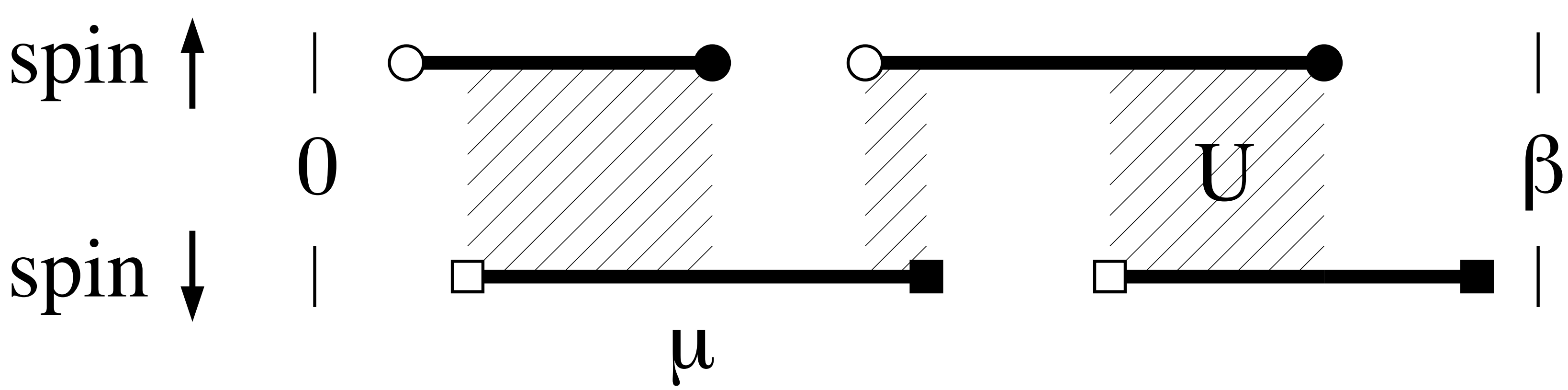

$$w_{\text{Hubbard}}(\{O_i(\tau_i)\}) \quad = \quad e^{\mu(l_\uparrow + l_\downarrow) - U l_{\text{overlap}}}$$
$$\times d\tau_1 \dots d\tau_{2n} \det M_\uparrow(V,\epsilon) M_\downarrow(V,\epsilon)$$

- $Tr_a[\dots]$ yields two determinants of hybridization matrices
- $Tr_c[\dots]$ must be computed explicitly ⟹ segment picture

Hybridization expansion

Werner & Millis, PRL (2007)

- Hybridization expansion for the Holstein-Hubbard model

$$H = \underbrace{H_{\text{loc}} + H_{\text{bath}}}_{H_1} + \underbrace{H_{\text{hyb}}}_{H_2}$$

$$H_{\text{loc}} = -\mu(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow + \lambda(n_\uparrow + n_\downarrow - 1)(b^\dagger + b) + \omega_0 b^\dagger b$$

$$H_{\text{bath}} = \sum_{p\sigma} \epsilon_p a^\dagger_{p\sigma} a_{p\sigma}$$

$$H_{\text{hyb}} = \sum_{p\sigma} V_{p\sigma} c^\dagger_\sigma a_{p\sigma} + h.c.$$

- Expand partition function in powers of $H_2 = H_{\text{hyb}}$
- Compute $Tr_c Tr_a Tr_b [\ldots]$

Hybridization expansion

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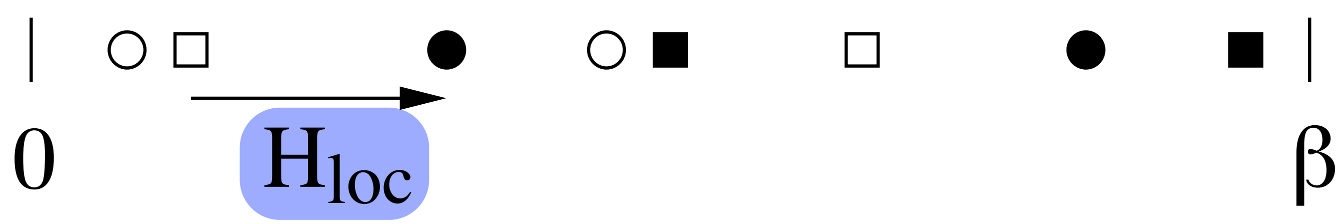

$$w_{\text{Holstein-Hubbard}}(\{O_i(\tau_i)\}) = Tr_c Tr_b\left[e^{-\beta H_{\text{loc}}} O_{2n}(\tau_{2n})\ldots O_1(\tau_1)\right]$$
$$\times d\tau_1 \ldots d\tau_{2n} \det M_\uparrow(V,\epsilon) M_\downarrow(V,\epsilon)$$

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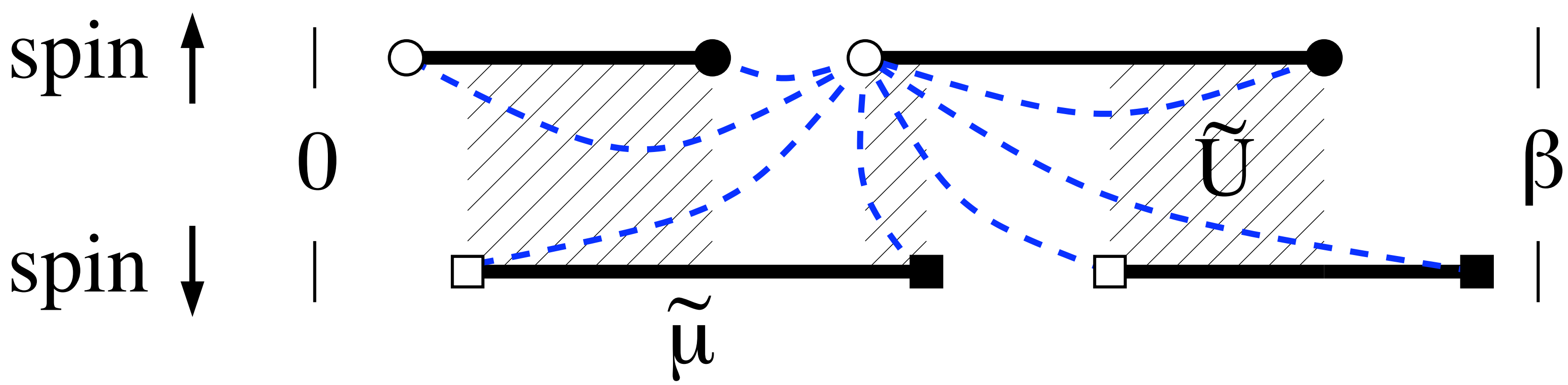


$$w_{\text{Holstein-Hubbard}}(\{O_i(\tau_i)\}) = Tr_c Tr_b\left[e^{-\beta H_{\text{loc}}} O_{2n}(\tau_{2n})\ldots O_1(\tau_1)\right]$$
$$\times d\tau_1 \ldots d\tau_{2n} \det M_\uparrow(V,\epsilon) M_\downarrow(V,\epsilon)$$

$$= w_{\text{phonon}}(\{O_i(\tau_i)\}) Tr_c\left[e^{-\beta \tilde{H}^{\text{Hubbard}}_{\text{loc}}} O_{2n}(\tau_{2n})\ldots O_1(\tau_1)\right]$$
$$\times d\tau_1 \ldots d\tau_{2n} \det M_\uparrow(V,\epsilon) M_\downarrow(V,\epsilon)$$

Holstein phonons

Werner & Millis, PRL (2007)

- Decouple electrons and phonons by Lang-Firsov transformation

$$H_{\text{loc}} = -\mu(n_\uparrow + n_\downarrow) + Un_\uparrow n_\downarrow + \lambda(n_\uparrow + n_\downarrow - 1)\sqrt{2}X + \frac{\omega_0}{2}(X^2 + P^2)$$

$$X = \frac{b^\dagger + b}{\sqrt{2}}, P = \frac{b^\dagger - b}{i\sqrt{2}}, [P, X] = i$$

- Shift X by $X_0 = (\sqrt{2}\lambda/\omega_0)(n_\uparrow + n_\downarrow - 1)$ using e^{iPX_0}

$$\tilde{H}_{\text{loc}} = e^{iPX_0} H_{\text{loc}} e^{-iPX_0} = \underbrace{-\tilde{\mu}(n_\uparrow + n_\downarrow) + \tilde{U} n_\uparrow n_\downarrow}_{\tilde{H}_{\text{loc}}^{\text{Hubbard}}} + \frac{\omega_0}{2}(X^2 + P^2)$$

$$\begin{aligned} \tilde{\mu} &= \mu - \lambda^2/\omega_0 \\ \tilde{U} &= U - 2\lambda^2/\omega_0 \\ \tilde{c}_\sigma &= e^{-\frac{\lambda}{\omega_0}(b^\dagger - b)} c_\sigma \end{aligned}$$

$$\Downarrow$$

$$\tilde{w}_{\text{Hubbard}}(\{O_i(\tau_i)\})$$

Holstein phonons

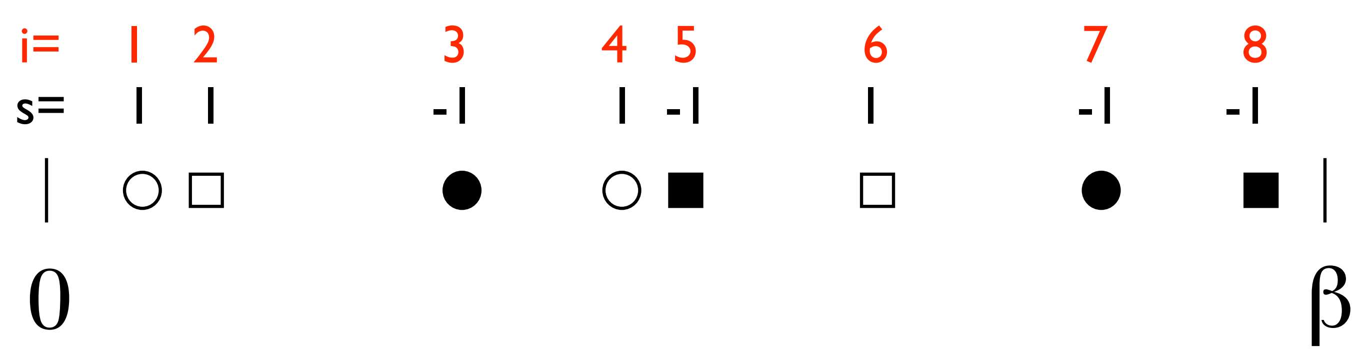
Werner & Millis, PRL (2007)

- Phonon contribution

$$w_{\text{phonon}}(\{O_i(\tau_i)\}) = \left\langle e^{s_{2n}A(\tau_{2n})} \ldots e^{s_1 A(\tau_1)} \right\rangle_b$$

$$A(\tau) = \frac{\lambda}{\omega_0}(e^{\omega_0 \tau} b^\dagger - e^{-\omega_0 \tau} b)$$

$$w_{\text{phonon}}(\{O_i(\tau_i)\}) = \exp\left[-\frac{\lambda^2}{\omega_0^2} \frac{1}{\sinh(\frac{\beta\omega_0}{2})} \left\{ n \cosh\left(\frac{\beta\omega_0}{2}\right) + \sum_{2n \geq i > j \geq 1} s_i s_j \cosh\left(\left(\frac{\beta}{2} - (\tau_i - \tau_j)\right)\omega_0\right) \right\} \right]$$



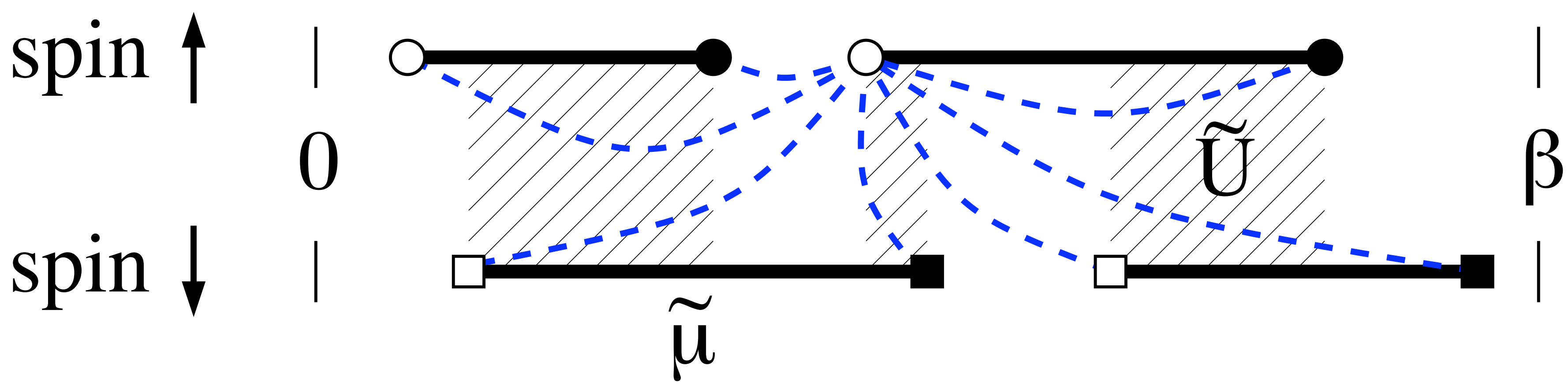
Holstein phonons

Werner & Millis, PRL (2007)

- Total weight

$$w_{\text{Holstein-Hubbard}}(\{O_i(\tau_i)\}) = \tilde{w}_{\text{Hubbard}}(\{O_i(\tau_i)\})w_{\text{phonon}}(\{O_i(\tau_i)\})$$

- Phonons yield additional (nonlocal) interaction between segment end points

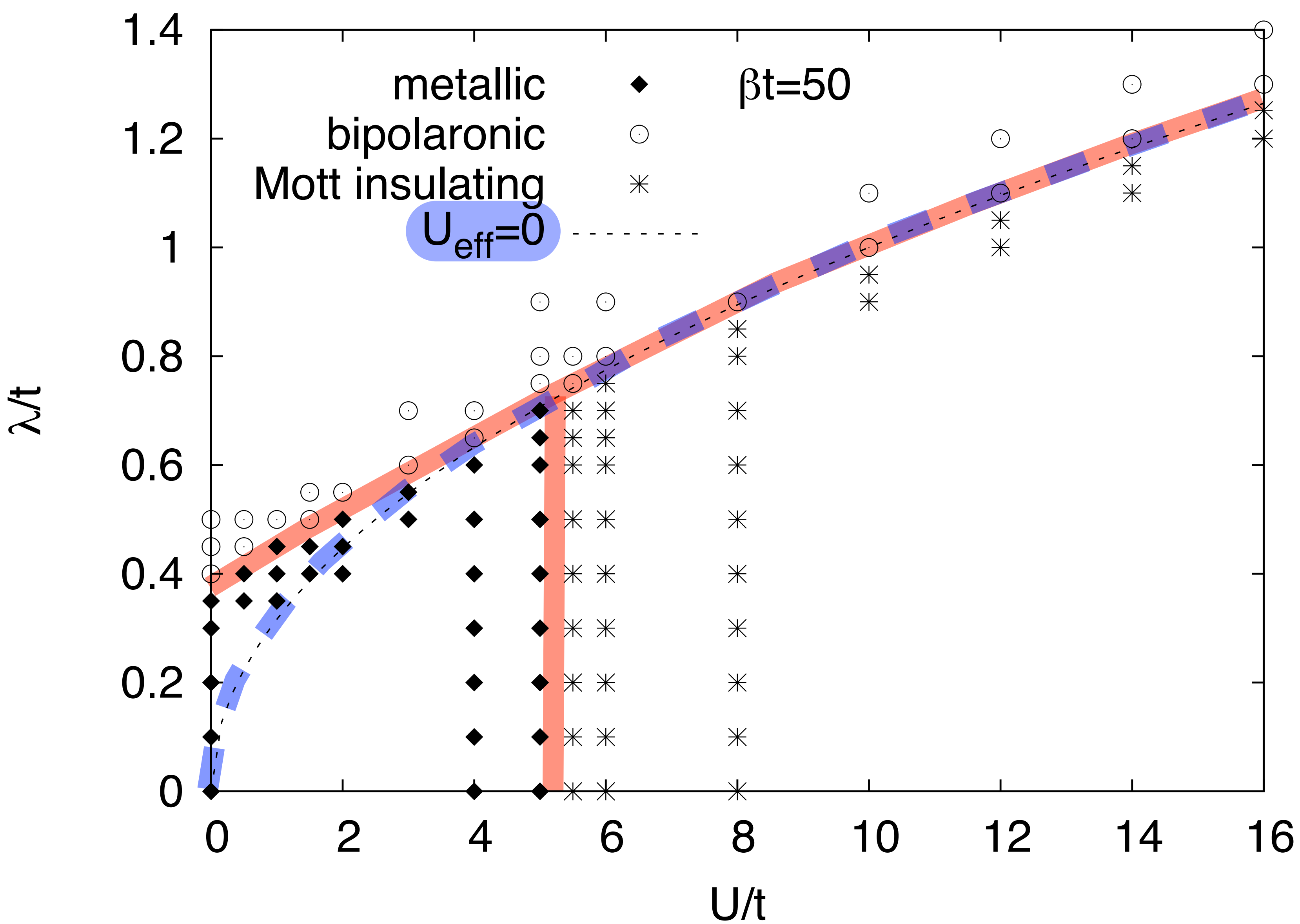


Holstein phonons

Werner & Millis, PRL (2007)

- Phasediagram

$$\text{bandwidth} = 4, \quad \omega_0 = 0.2$$



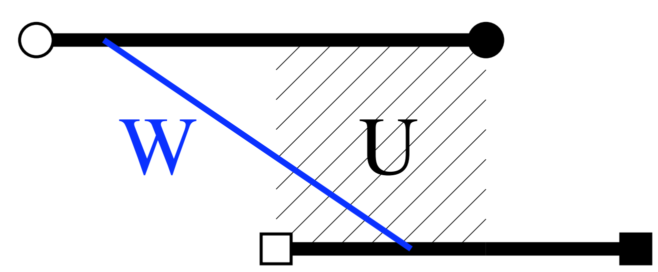
Frequency dependent *U*

Werner & Millis, in preparation

- Arbitrary nonlocal (screened) interactions

$$w_{\text{int}} = \exp\left[-\sum_{\alpha\neq\beta}\int_0^\beta d\tau U_{\alpha\beta} n_\alpha(\tau) n_\beta(\tau) -\frac{1}{2}\sum_{\alpha,\beta}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 W_{\alpha\beta}(\tau_1-\tau_2) n_\alpha(\tau_1) n_\beta(\tau_2)\right]$$

- Contribution from one pair of segments



$$\int_{\tau_1^s}^{\tau_1^e} d\tau_1 \int_{\tau_2^s}^{\tau_2^e} d\tau_2 W(\tau_1-\tau_2) = -H(\tau_1^e-\tau_2^e)+H(\tau_1^e-\tau_2^s)+H(\tau_1^s-\tau_2^e)-H(\tau_1^s-\tau_2^s)$$

$$H''(\tau) = W(\tau)$$

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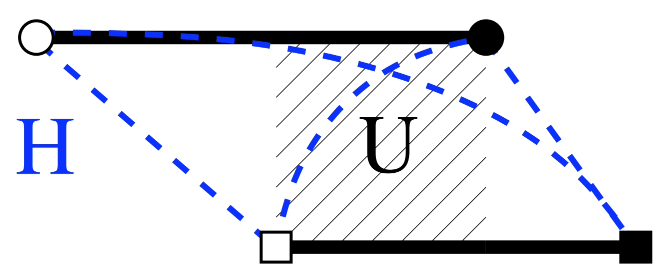

$$\int_{\tau_1^s}^{\tau_1^e} d\tau_1 \int_{\tau_2^s}^{\tau_2^e} d\tau_2 W(\tau_1-\tau_2) = -H(\tau_1^e-\tau_2^e) + H(\tau_1^e-\tau_2^s) + H(\tau_1^s-\tau_2^e) - H(\tau_1^s-\tau_2^s)$$

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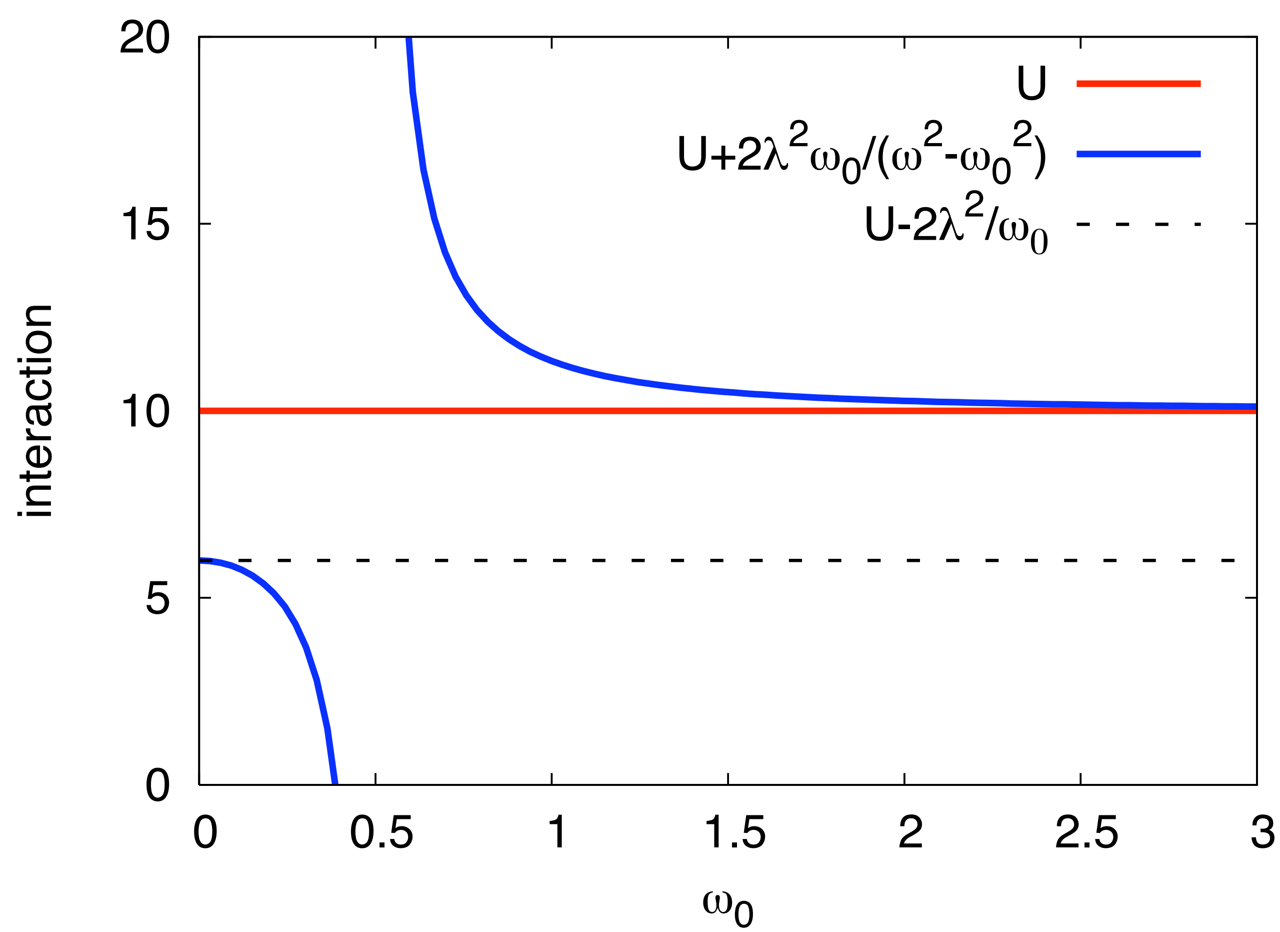
Frequency dependent *U*

Werner & Millis, in preparation

- Comparison with Holstein-Hubbard model yields

$$W_{\text{Holstein-Hubbard}}(\tau) = -\lambda^2 \frac{\cosh((\beta/2-\tau)\omega_0)}{\sinh(\beta\omega_0/2)}$$

$$W_{\text{Holstein-Hubbard}}(\omega) = \frac{2\lambda^2\omega_0}{\omega^2-\omega_0^2}$$



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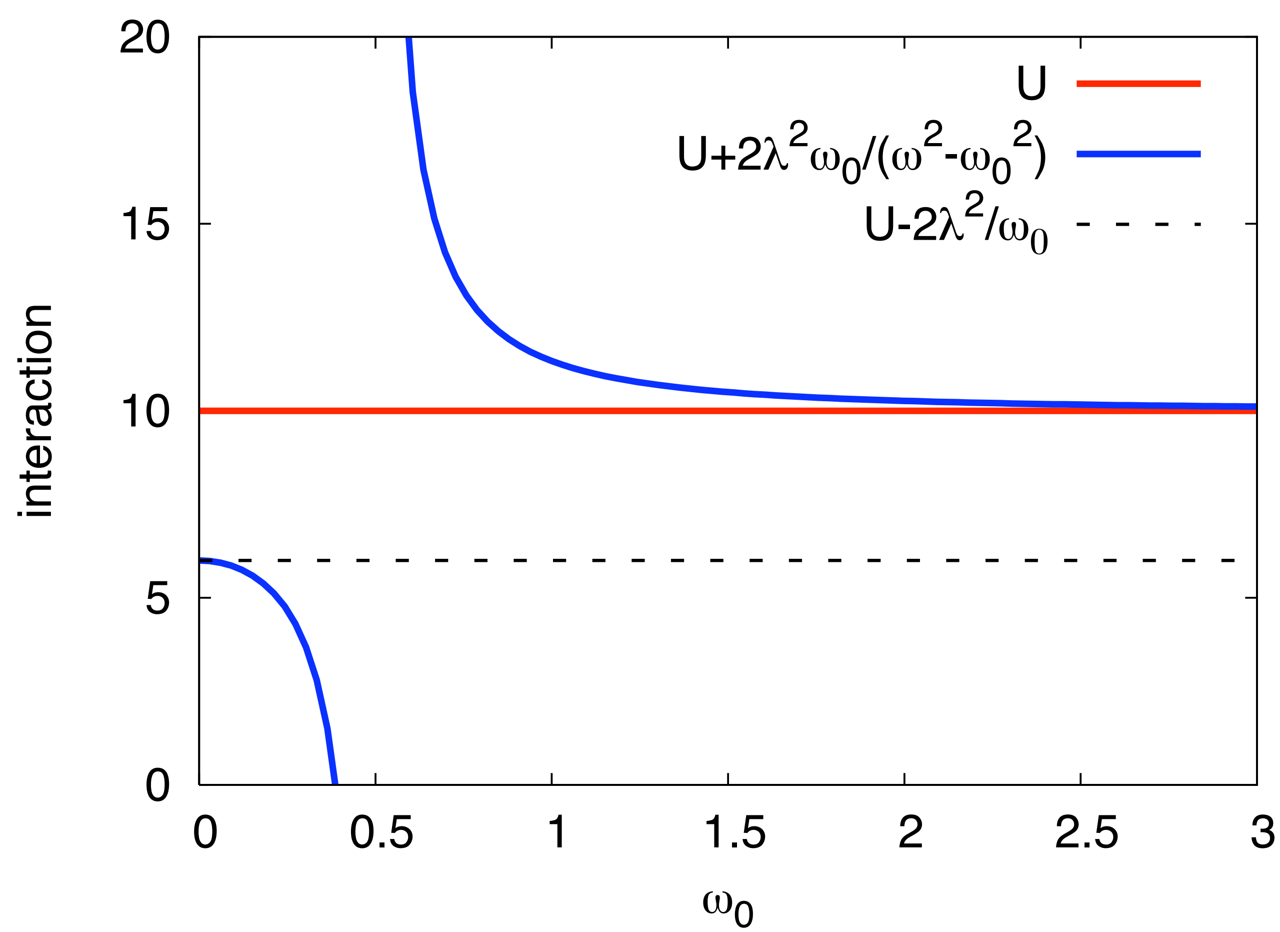

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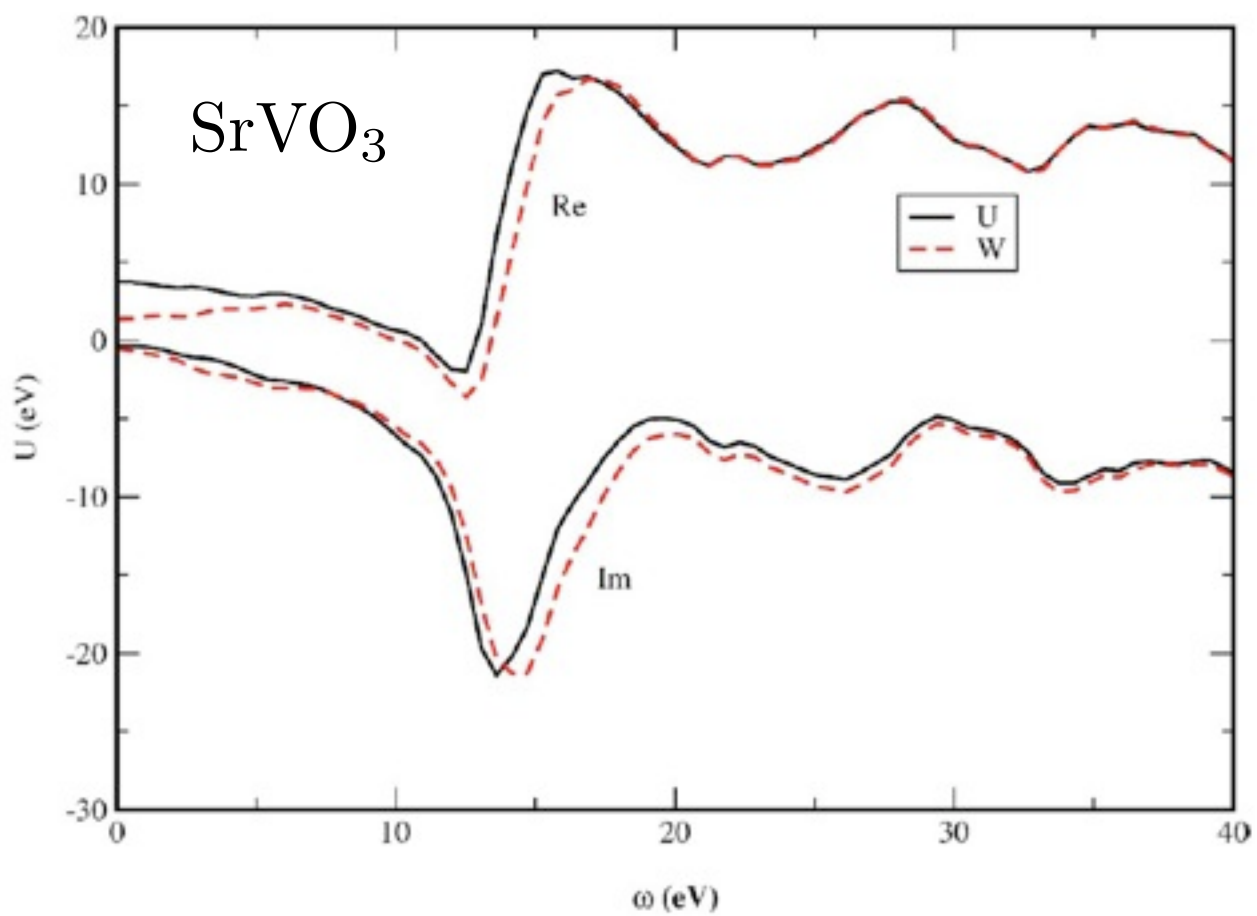


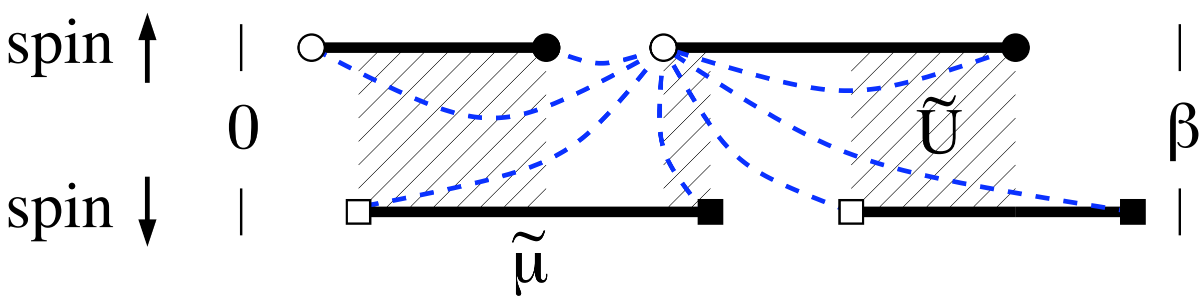
Aryasetiawan et al., PRB (2004)

Frequency dependent U

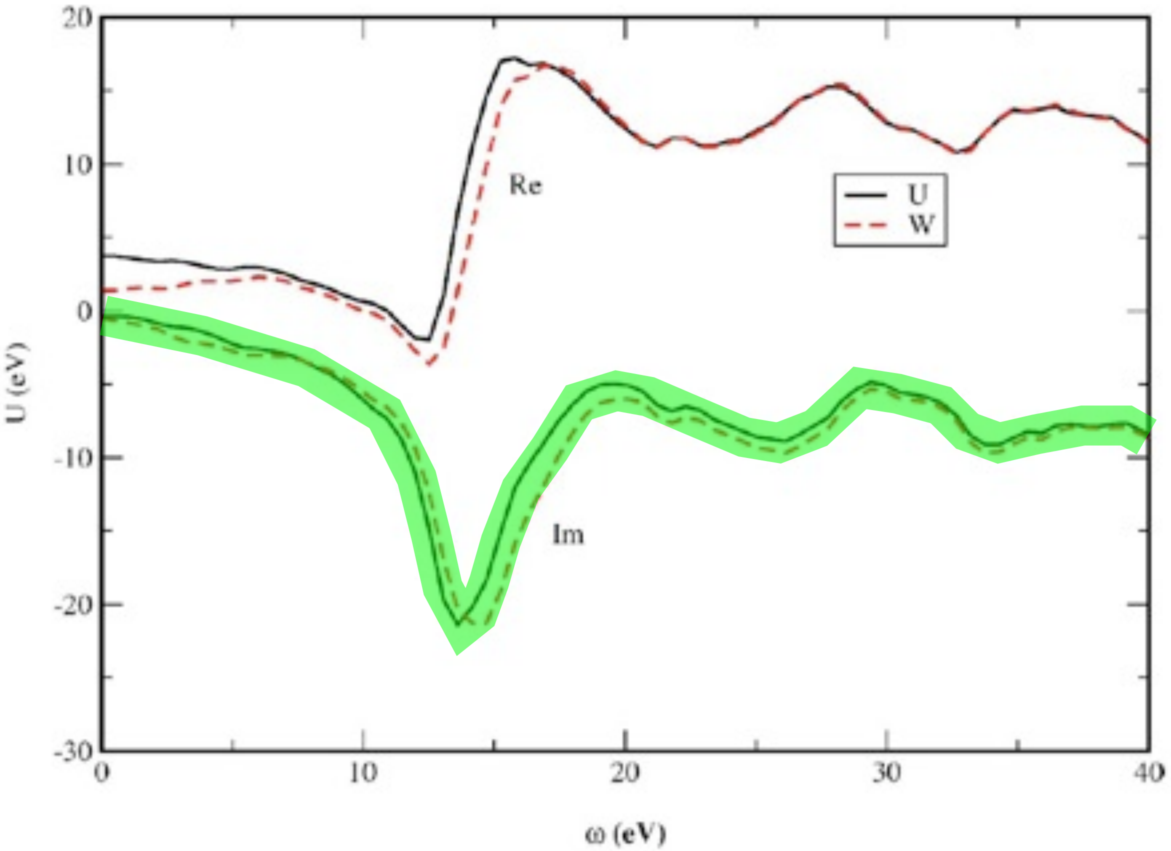
Werner & Millis, in preparation

- Non-local interaction for arbitrary $\mathrm{Im}[W(\omega)]$

$$W(\tau) = \int_0^\infty d\omega \frac{\mathrm{Im}[W(\omega)]}{\pi} \frac{\cosh((\beta/2-\tau)\omega)}{\sinh(\beta\omega/2)}$$



Werner & Millis, PRL (2007)

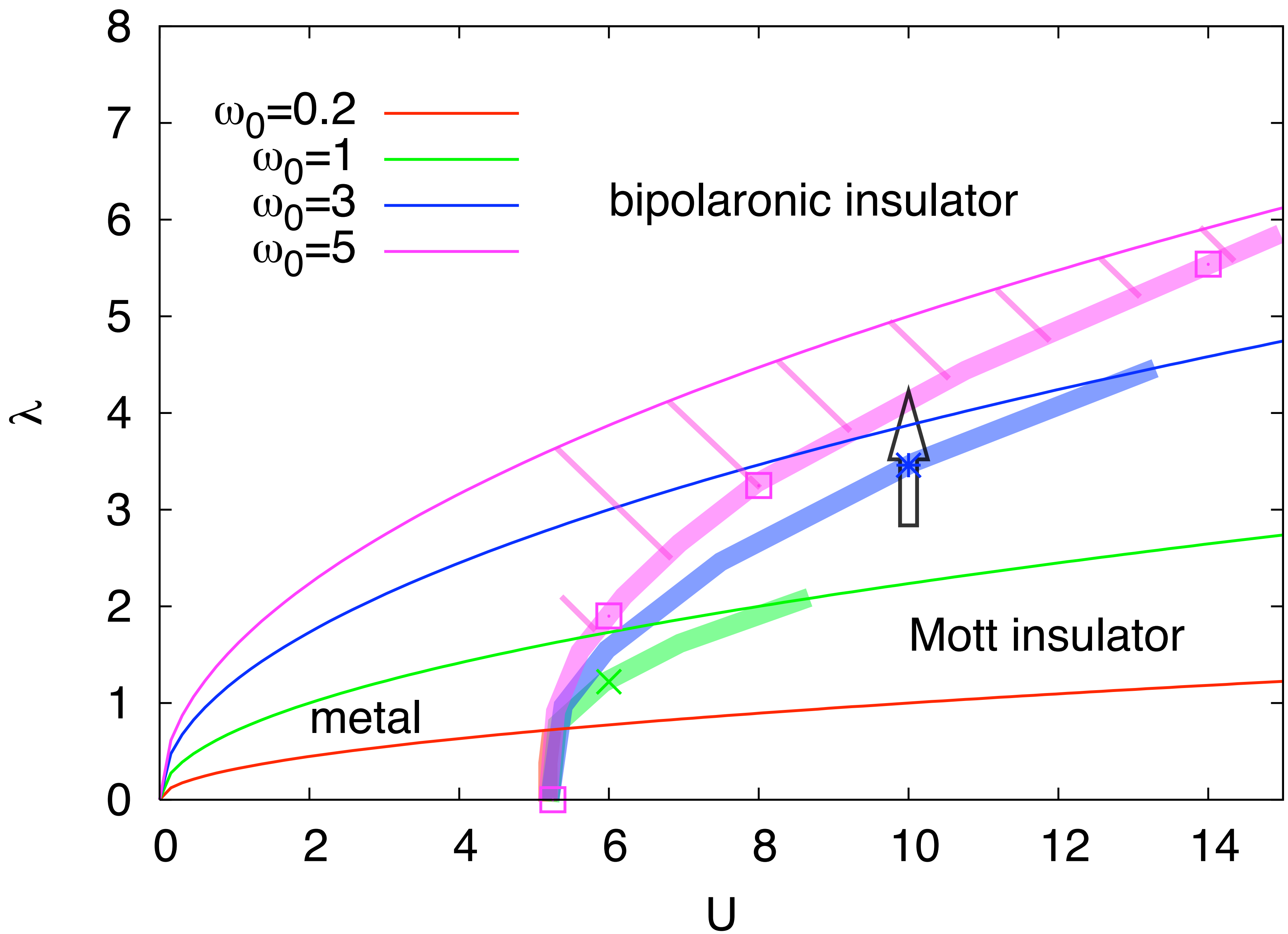


Aryasetiawan et al., PRB (2004)

Metal-insulator transition

Werner & Millis, in preparation

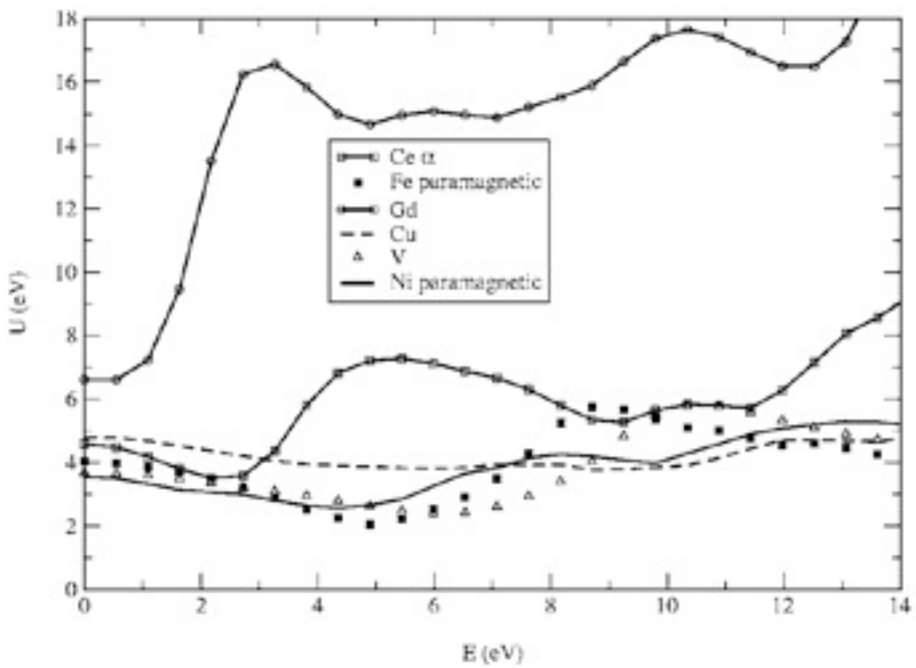
- Holstein-Hubbard model with $\omega_0 \sim \mathrm{bandwidth}$
- Insulator-metal transition at $U \gg U_{c2}$ induced by increasing λ

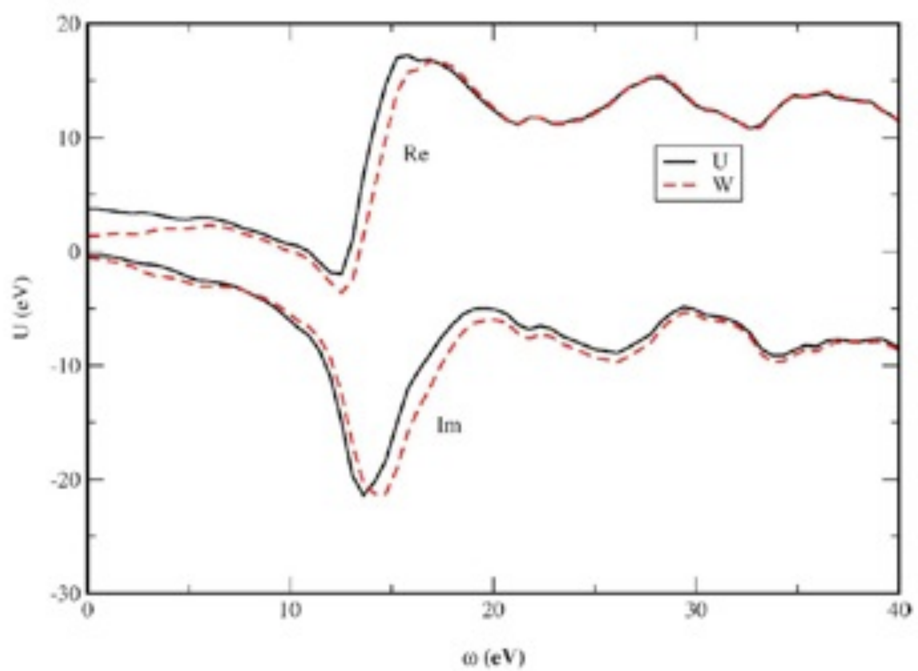


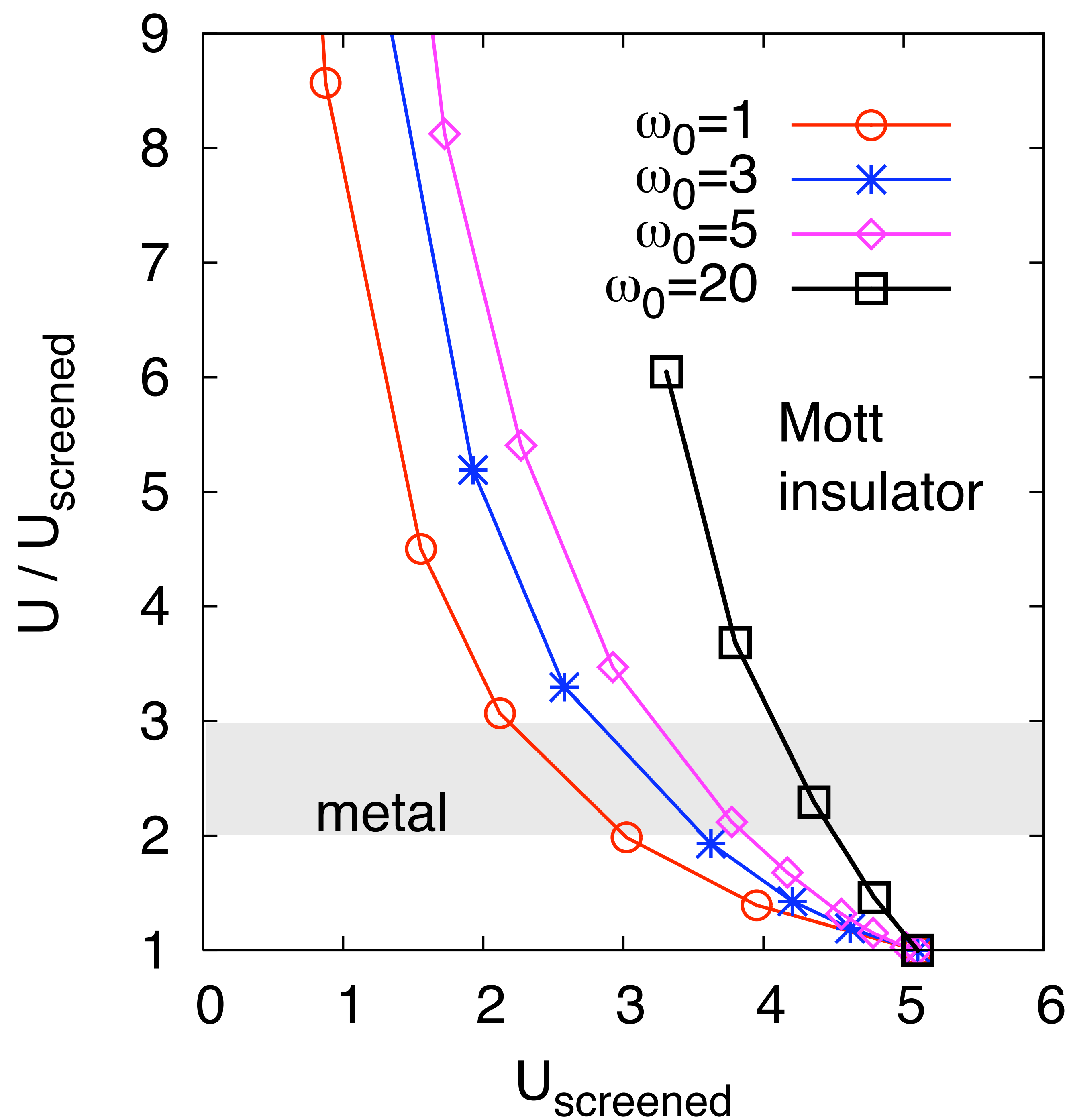
Metal-insulator transition

Werner & Millis, in preparation

- Screening effect on U_{c2} non-negligible even for $\omega_0 \gg \mathrm{bandwidth}$



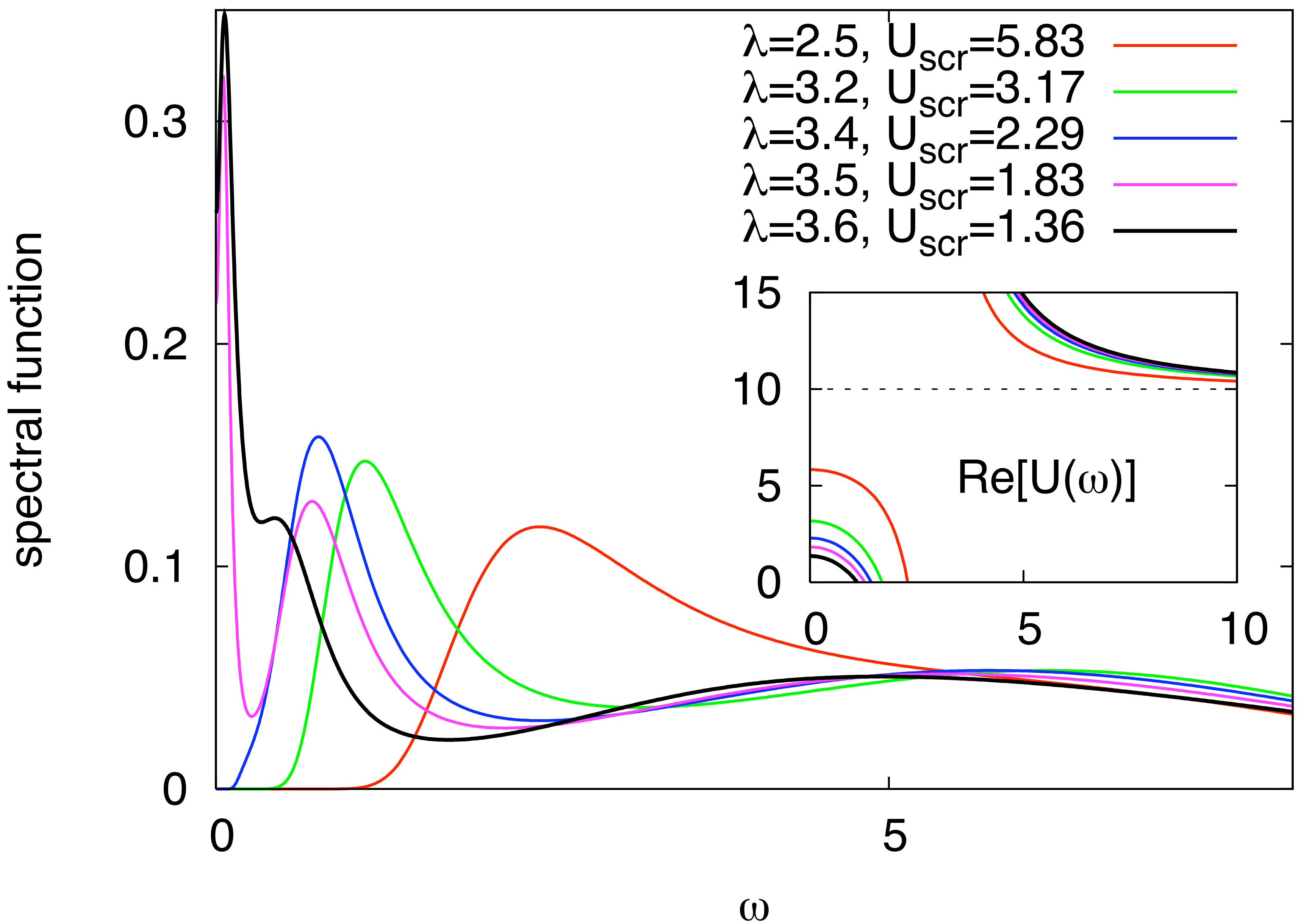




Metal-insulator transition

Werner & Millis, in preparation

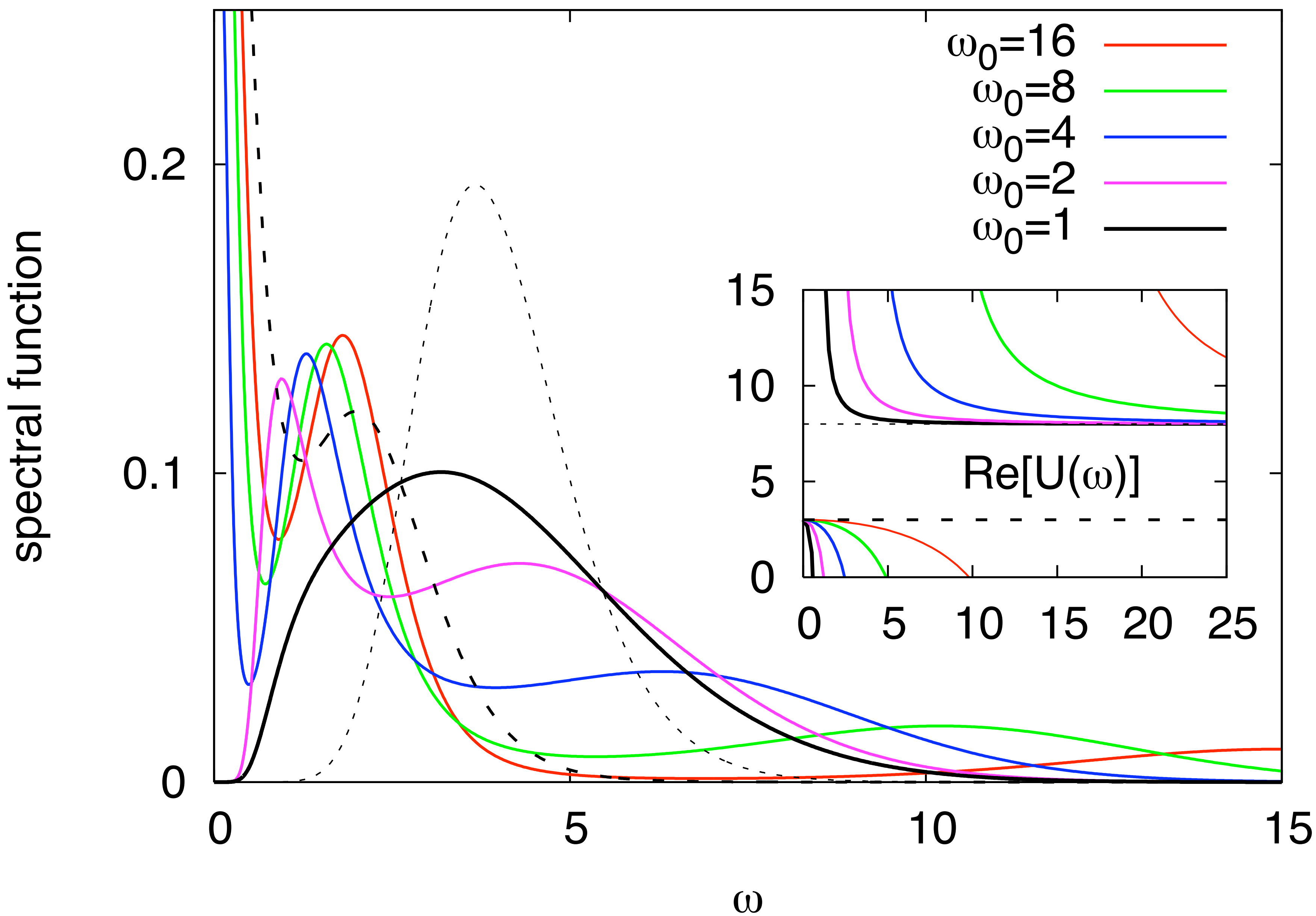
- $U_{\rm bare} = 10,\ \omega_0 = 3$
- spectral function has multi-peak structure
- as screening strength is increased the gap shrinks



Metal-insulator transition

Werner & Millis, in preparation

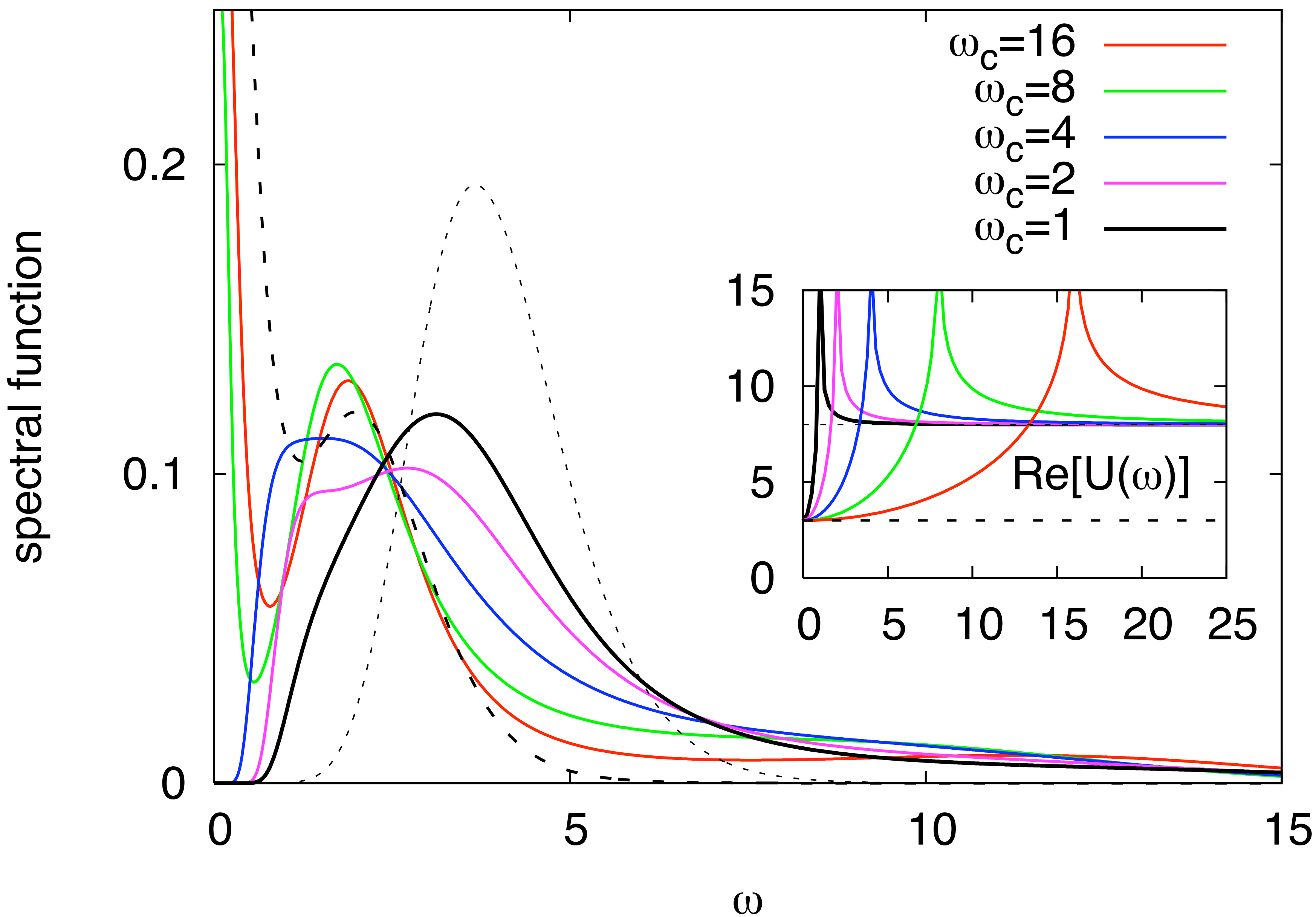
- $U_{\mathrm{bare}} = 8,\ U_{\mathrm{screened}} = 3$
- ``screened *U*'' and ``unscreened *U*'' Hubbard bands ...
- ... but no good estimate of $U_{\mathrm{bare}},\ U_{\mathrm{screened}}$ from spectral function



Metal-insulator transition

Werner & Millis, in preparation

- Same for ``Ohmic'' model: $\mathrm{Im}W(\omega) = -\alpha\pi\Theta(\omega^2 - \omega_c^2)$
- qualitatively similar to ``plasmon'' model
- broad high energy tail instead of ``unscreened *U*'' Hubbard bands



Summary

- Hybridization expansion for the Holstein-Hubbard model
- General formalism for frequency-dependent interactions
- Metal-insulator transition for $U \gg U_{c2}, \quad \omega_0 \sim \text{bandwidth}$
- Outlook: application to real materials, GW+DMFT, E-DMFT, ...