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Influence of Hund's rule coupling in correlated multi-orbital systems



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Influence of Hund's rule coupling in correlated multi-orbital systems

1. Why multi-orbital models?



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Influence of Hund's rule coupling in correlated multi-orbital systems

1. Why multi-orbital models?
2. How important is Hund's coupling – impurity point of view



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1. Why multi-orbital models?
2. How important is Hund's coupling – impurity point of view
3. The MIT in two-orbital Hubbard model



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4. **Conclusio**



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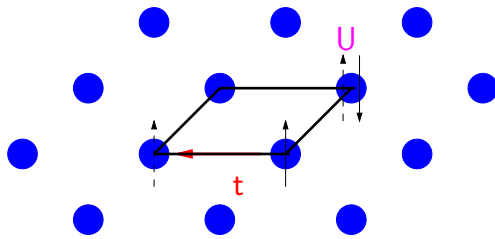


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Simplest possible model for TMO: **one-band Hubbard model**

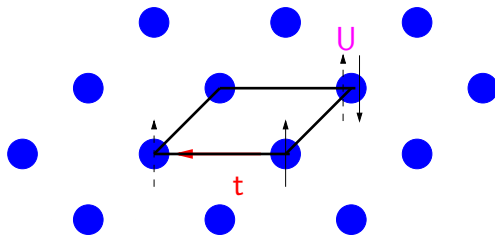


$$H = -t \sum_{\langle i,j \rangle \sigma} d_{i\sigma}^\dagger d_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i\bar{\sigma}}$$

$$n_{i\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$$



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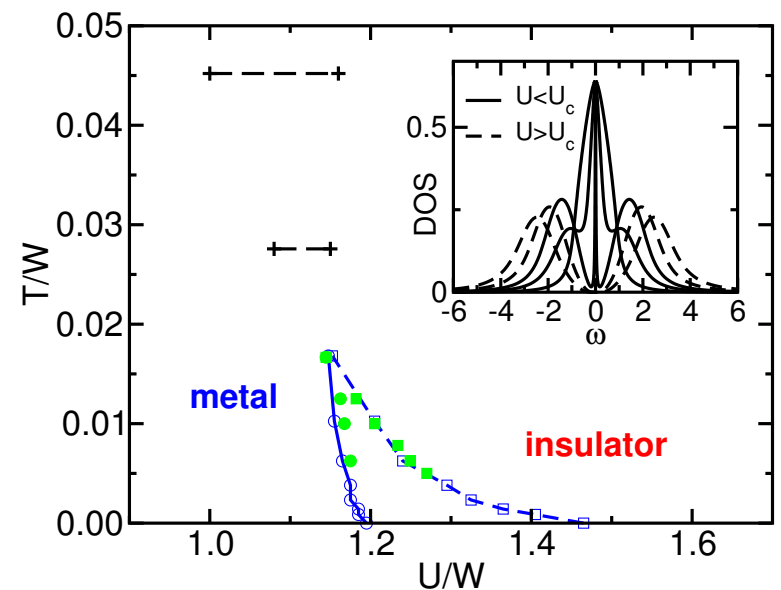


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Established properties (DMFT):

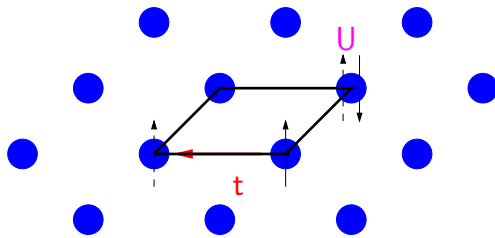
- Metal-insulator transition for $\langle n \rangle = 1$

Georges et al., RMP '96, Bulla et al., PRL '99 & PRB '01





Simplest possible model for TMO: **one-band Hubbard model**



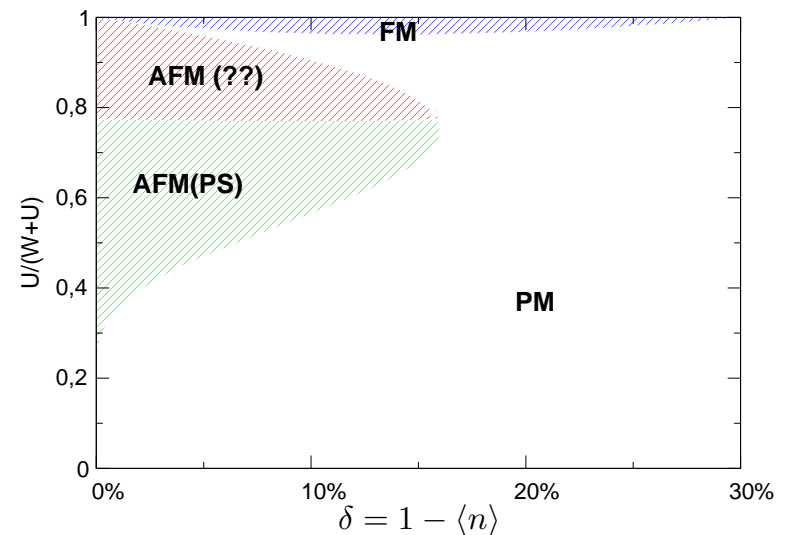
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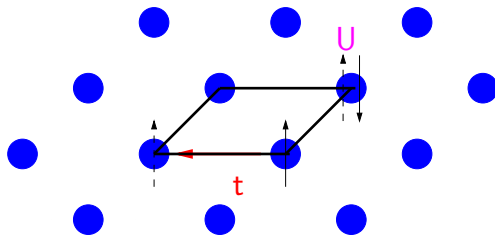
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- Magnetism (AFM & FM)

Zitzler et al., EPJ '02





Simplest possible model for TMO: **one-band Hubbard model**

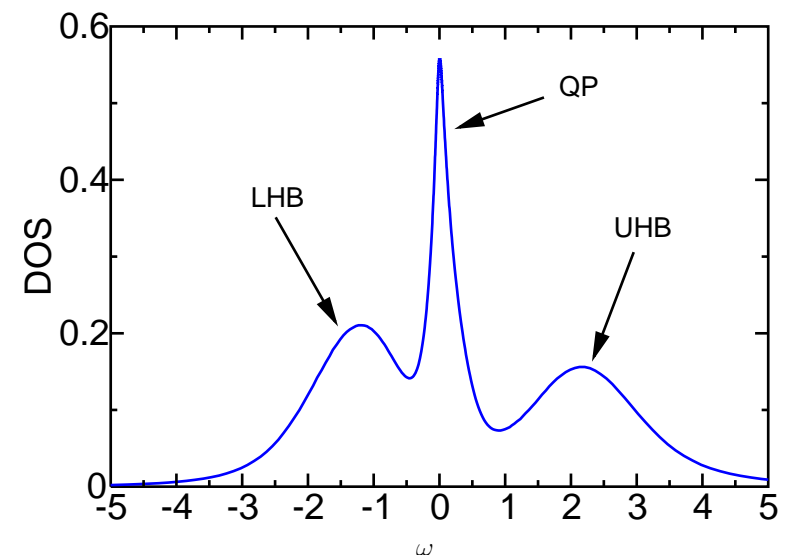


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Established properties (DMFT):

- Metal-insulator transition for $\langle n \rangle = 1$
- Magnetism (AFM & FM)
- Correlated metal for $\langle n \rangle < 1$

TP et al., PRB '93





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More realistic situation: Include orbital degrees of freedom

$$H = -t \sum_{\langle i,j \rangle m \sigma} d_{im\sigma}^\dagger d_{jm\sigma} + \frac{U}{2} \sum_{im\sigma} n_{im\sigma} n_{im\bar{\sigma}}$$



More realistic situation: Include orbital degrees of freedom

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direct Coulomb



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$$H = -t \sum_{\langle i,j \rangle m \sigma} d_{im\sigma}^\dagger d_{jm\sigma} + \frac{U}{2} \sum_{im\sigma} n_{im\sigma} n_{im\bar{\sigma}}$$
$$+ \frac{2U' - J_H}{4} \sum_{i, m \neq m'} \sum_{\sigma \sigma'} n_{im\sigma} n_{im'\sigma'}$$
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direct Coulomb

Hund's exchange



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$$- J_H \sum_{i, m \neq m'} \vec{S}_{im} \cdot \vec{S}_{im'}$$

Hund's exchange

+ ...

more complicated stuff



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How do we solve the impurity problem?



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How do we solve the impurity problem?

Wilson's numerical renormalization group:

Transform impurity Hamiltonian into “onion”

- Thicker outer shells \equiv high energy states
- Thin inner shells \equiv low energy states
- “Peel” onion successively \Rightarrow properties on successively lower energy scales





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👉 $T = 0$ & $T > 0$, exponentially small scales, DMFT



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Setup: $m = 2$, $\langle n \rangle = 2$, full $J_H \geq 0$, $U' = U - 2J_H$

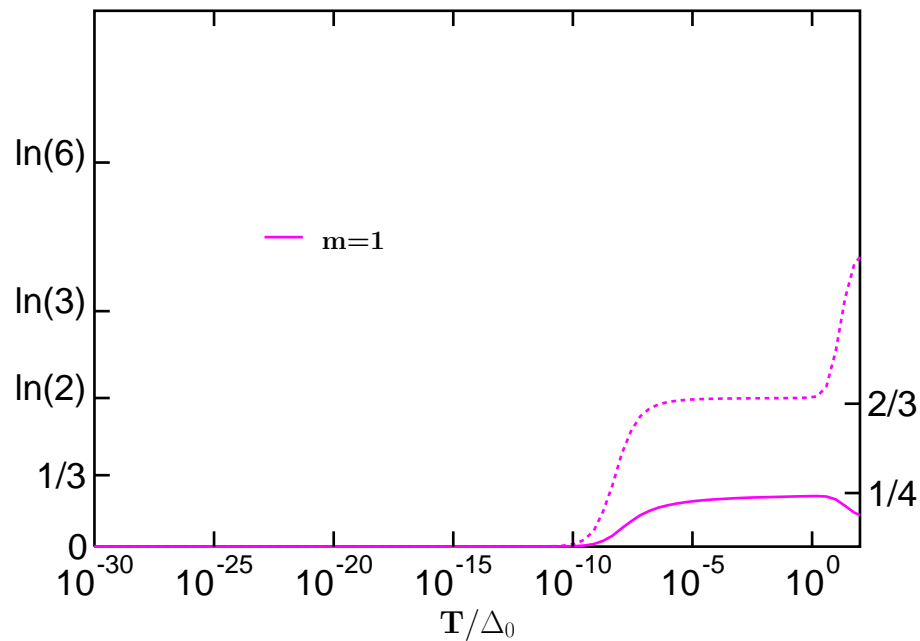
Δ_0 =coupling to fermionic baths, $U \gg \Delta_0$ ("Kondoregime")



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Thermodynamics

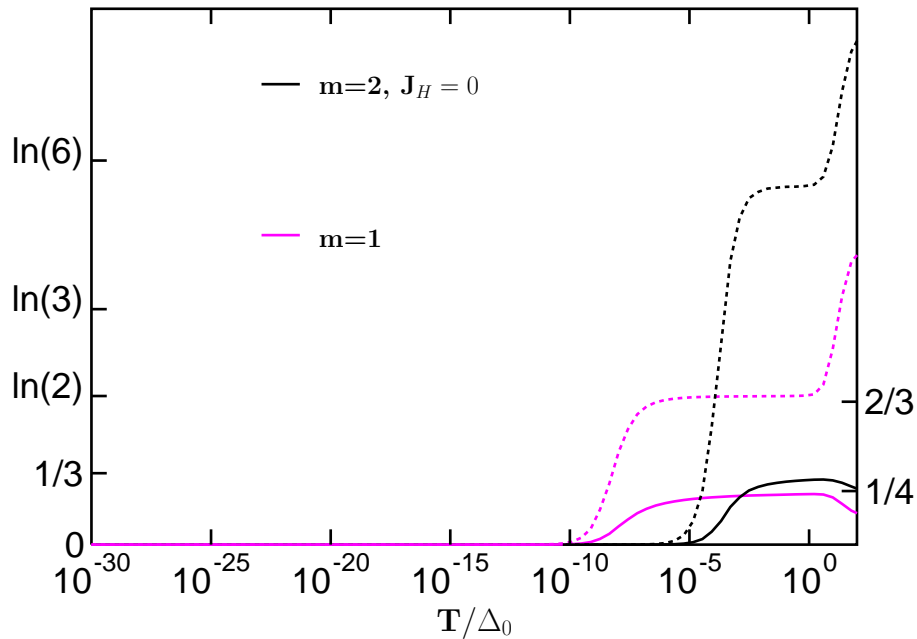




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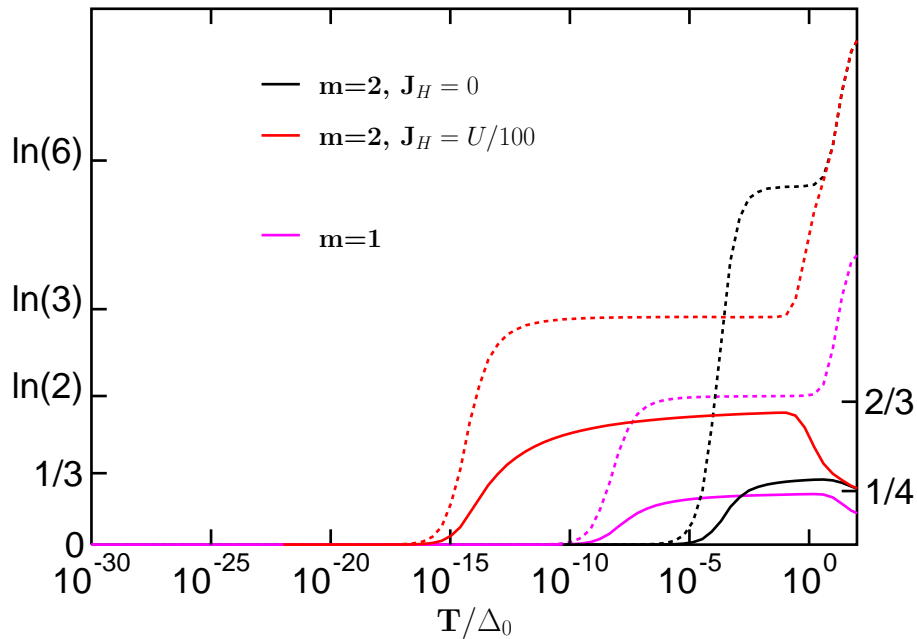




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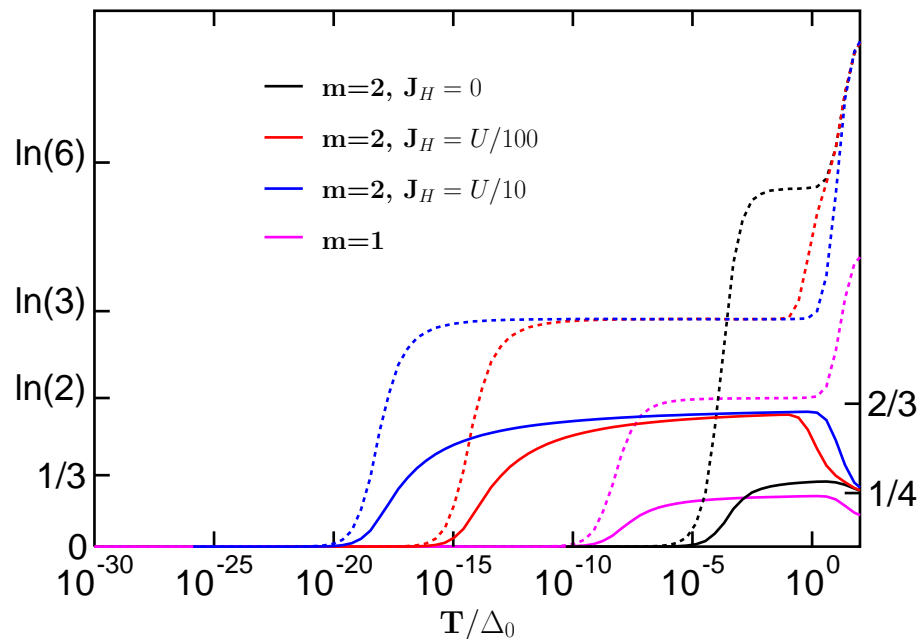




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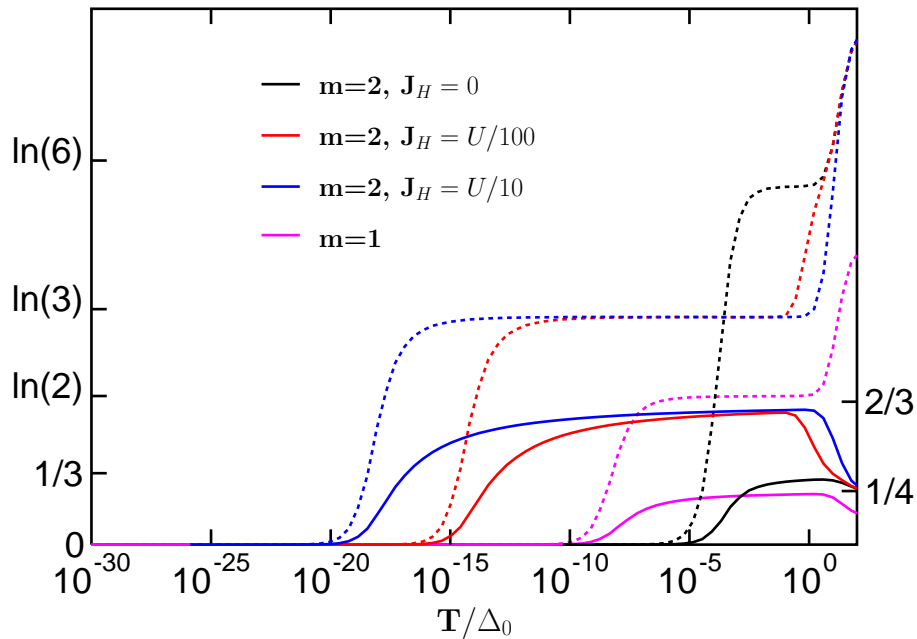




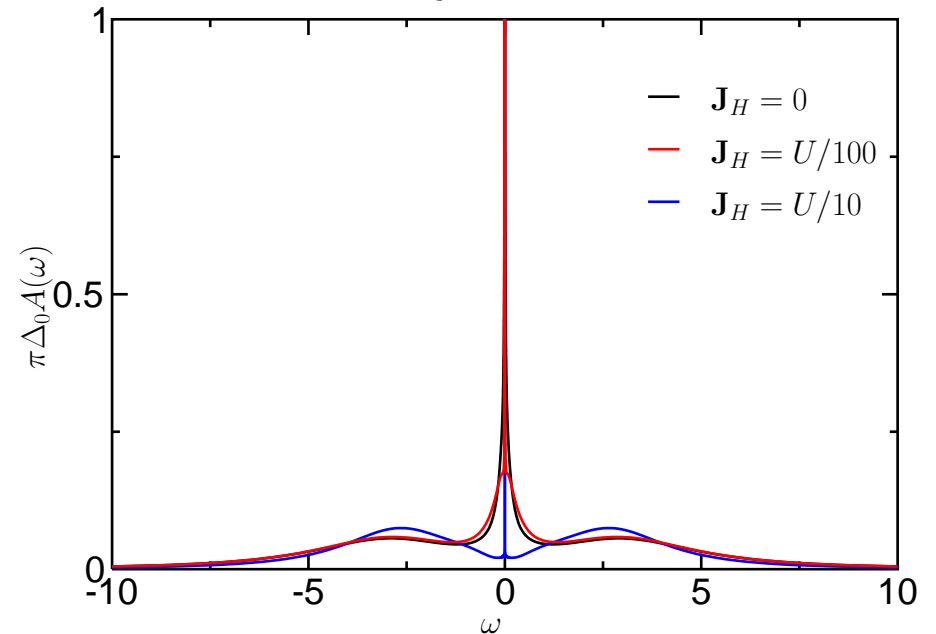
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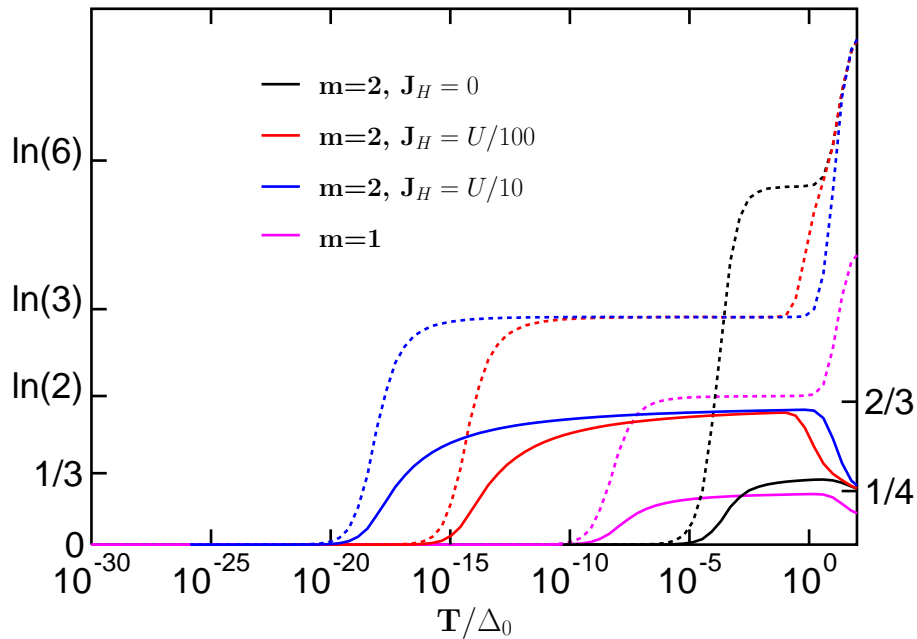




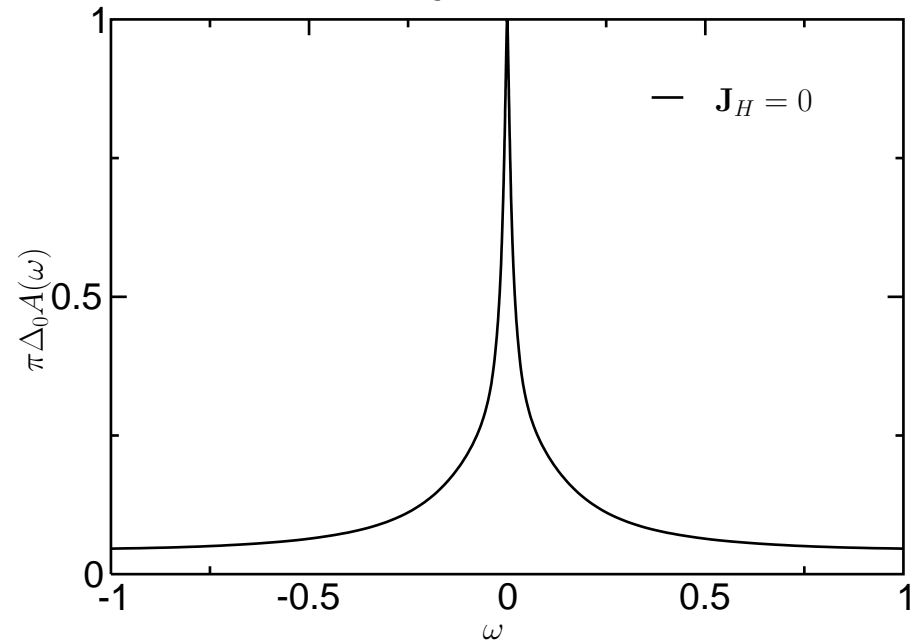
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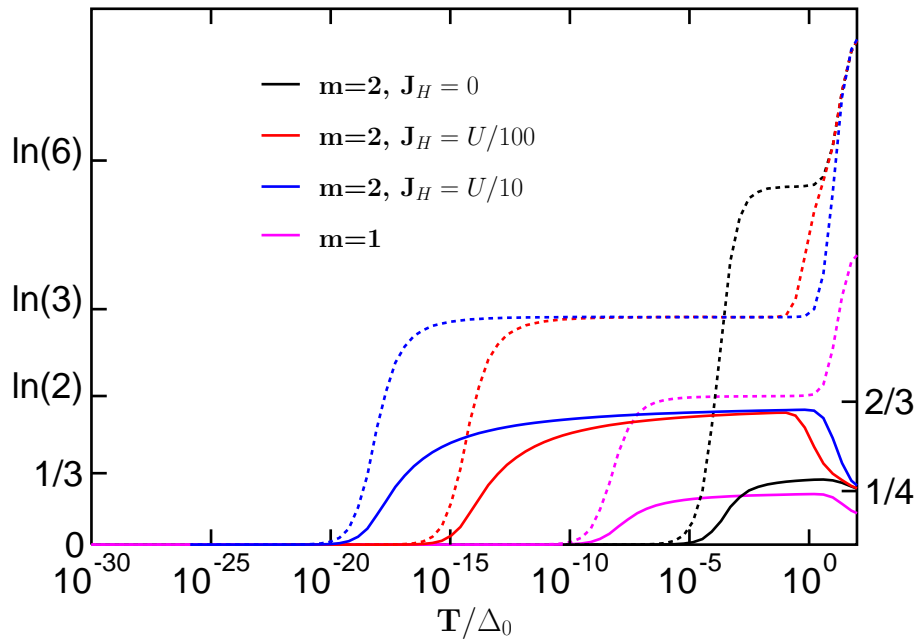




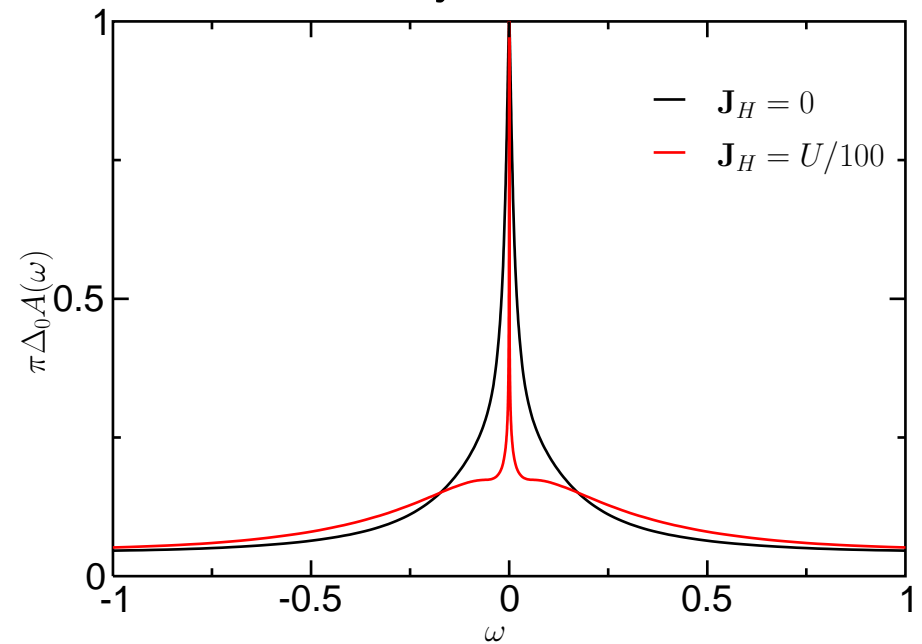
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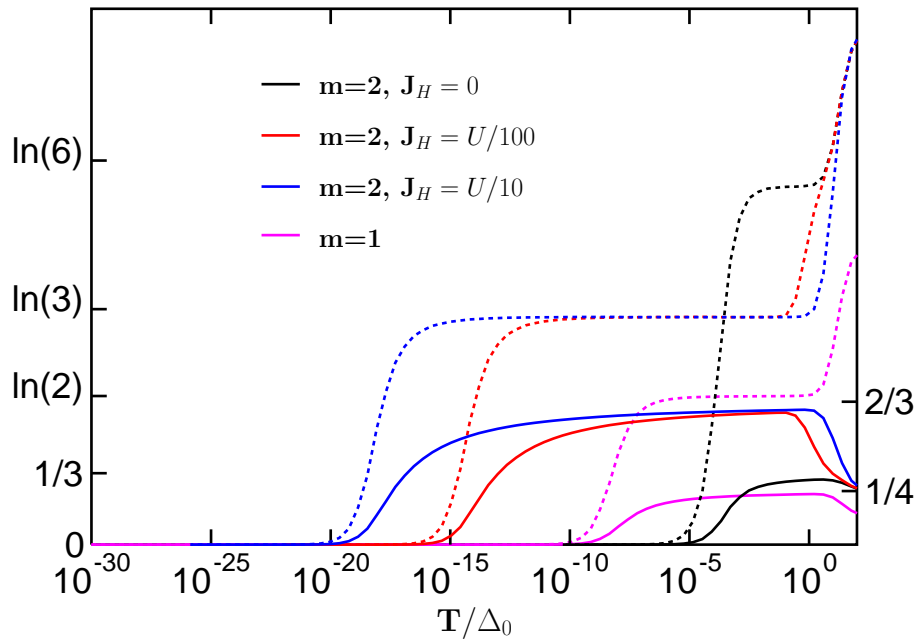




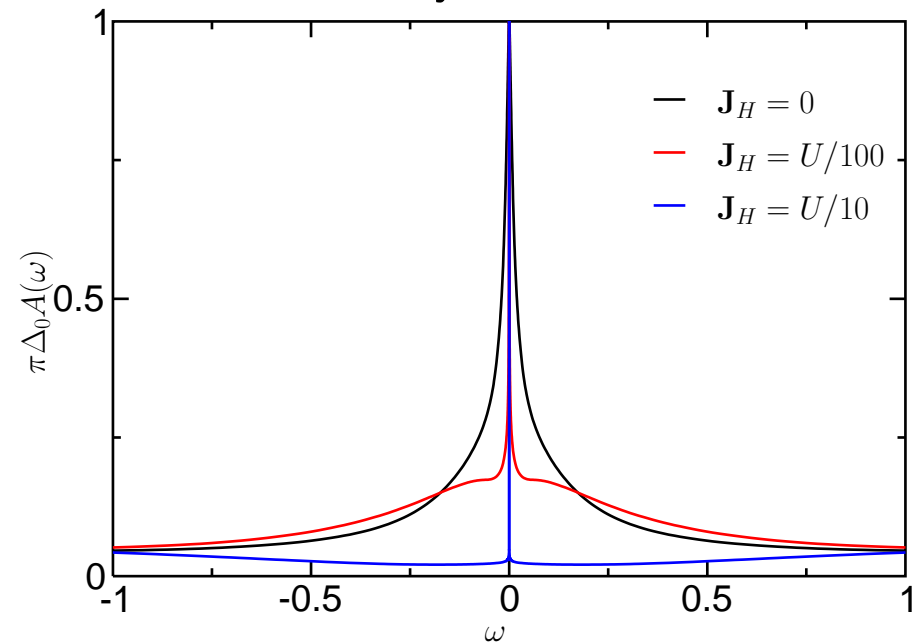
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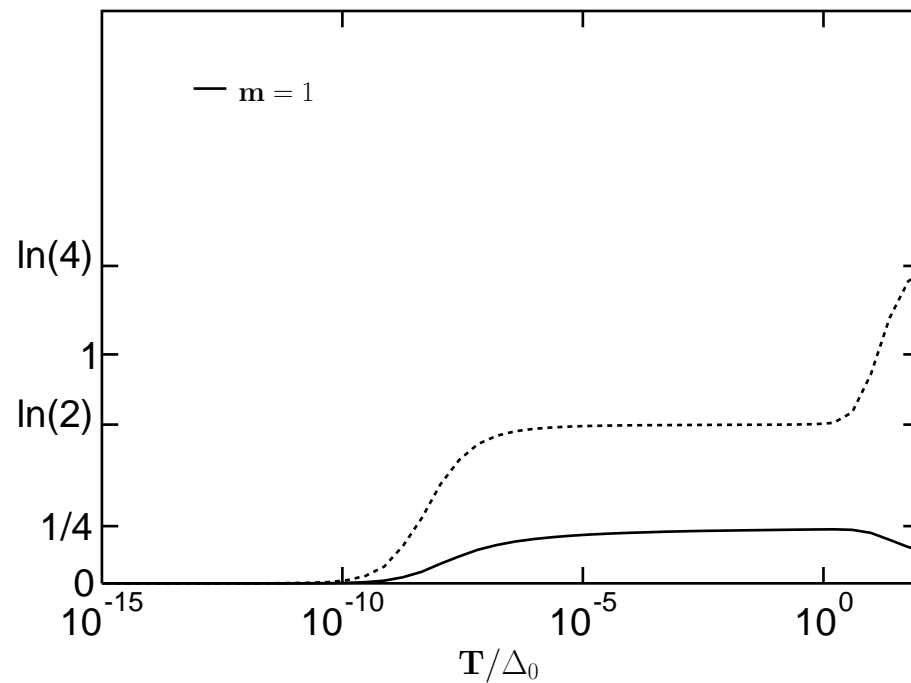
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Can one replace Hund's exchange by Ising part only?

TP & Bulla, EPJ B '05

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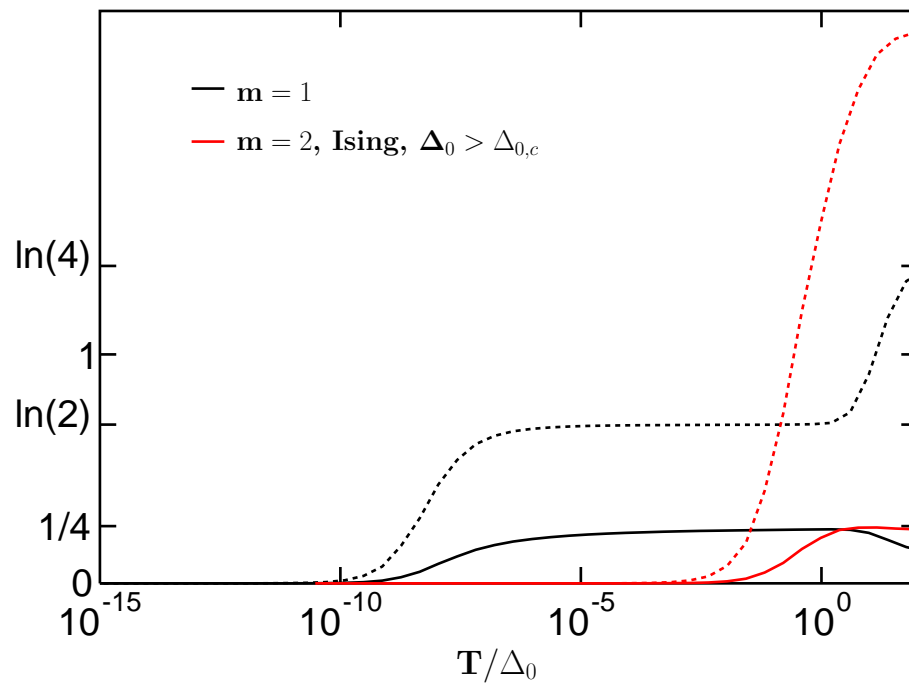




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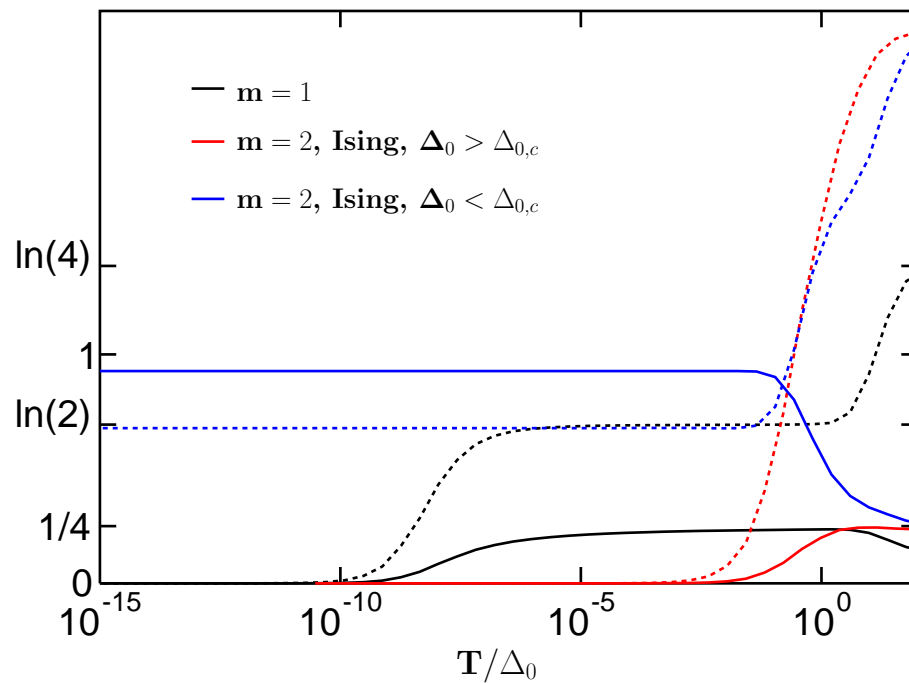




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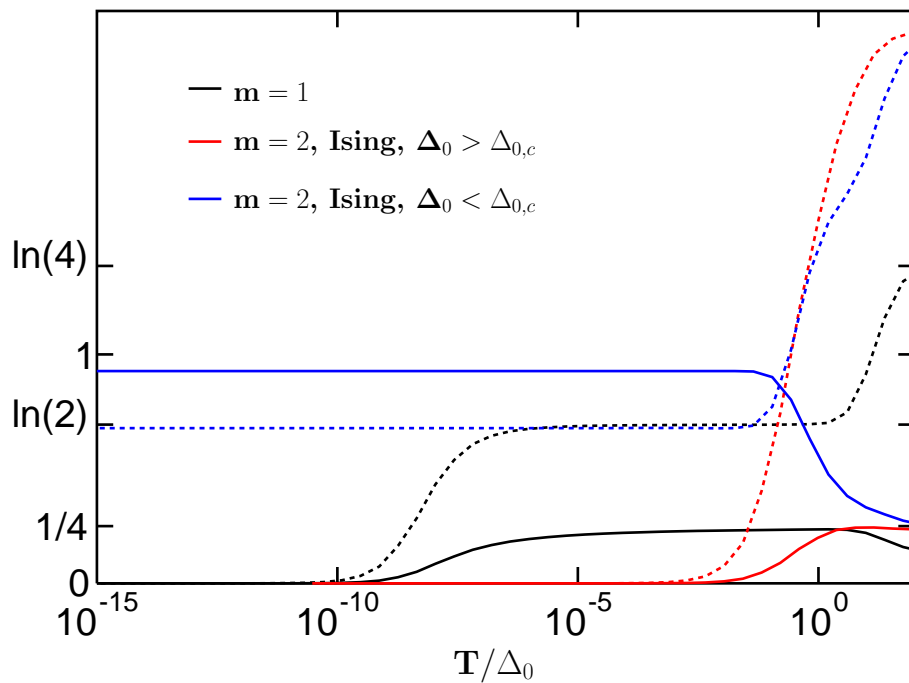




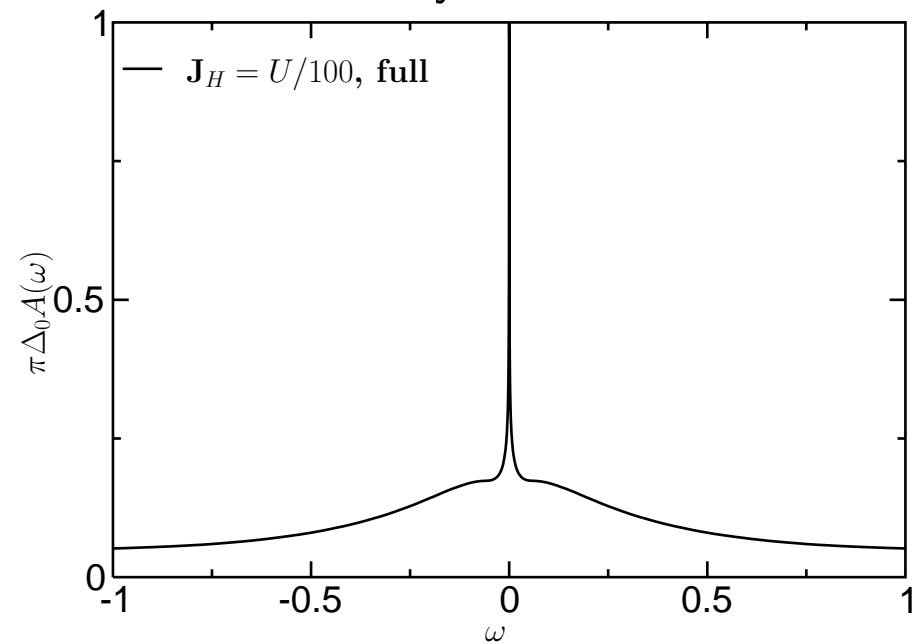
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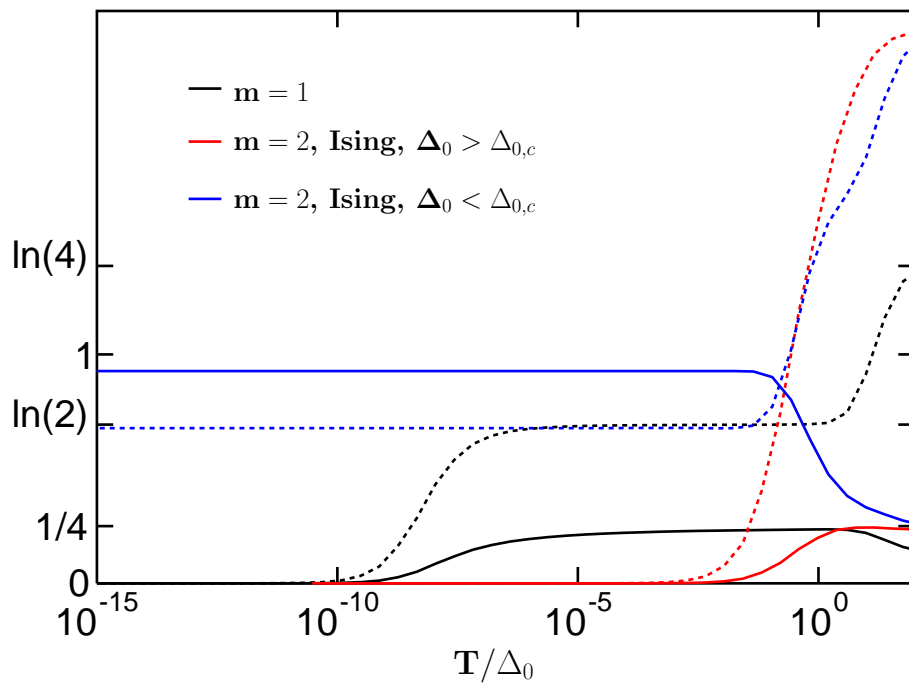




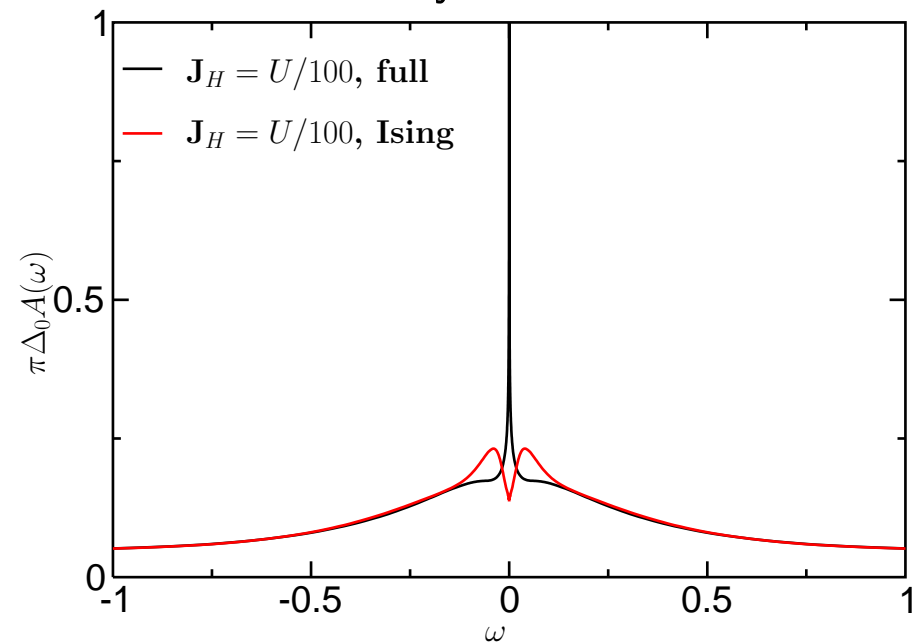
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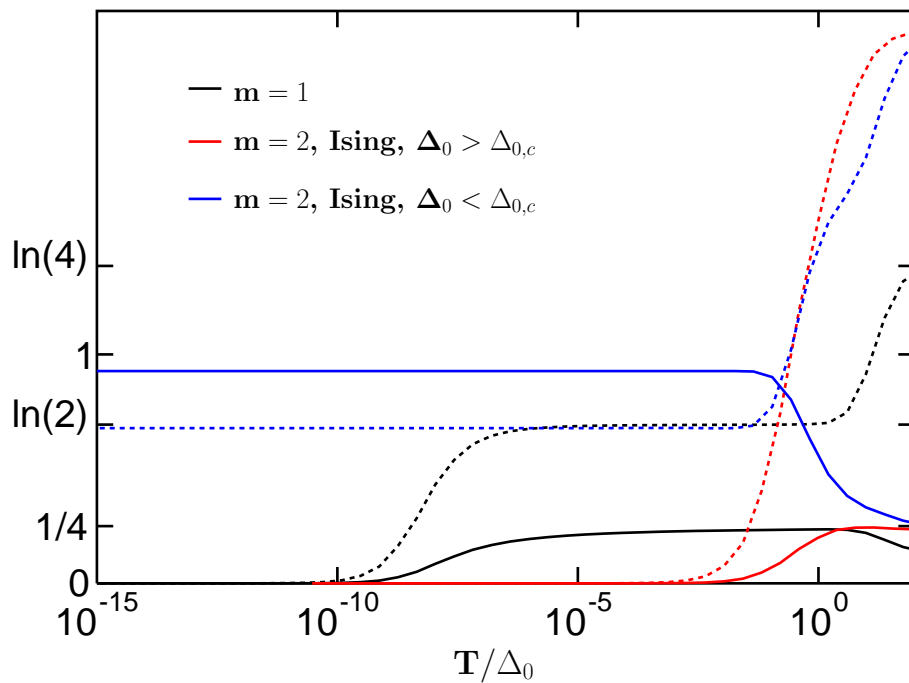




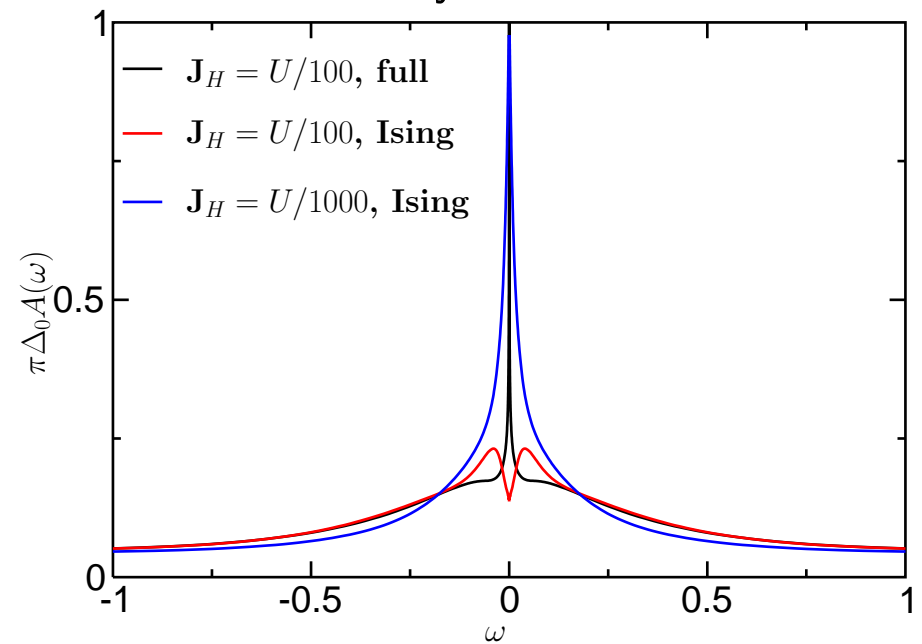
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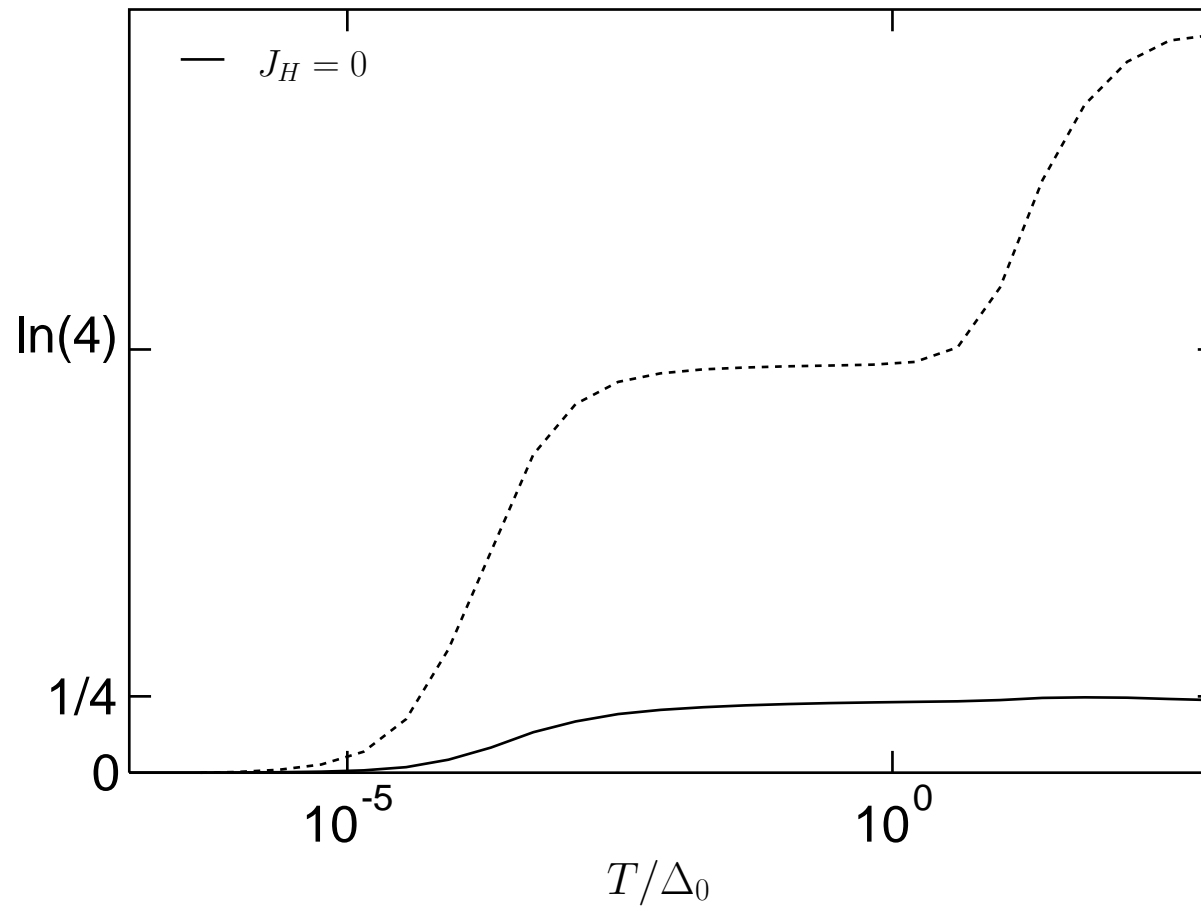


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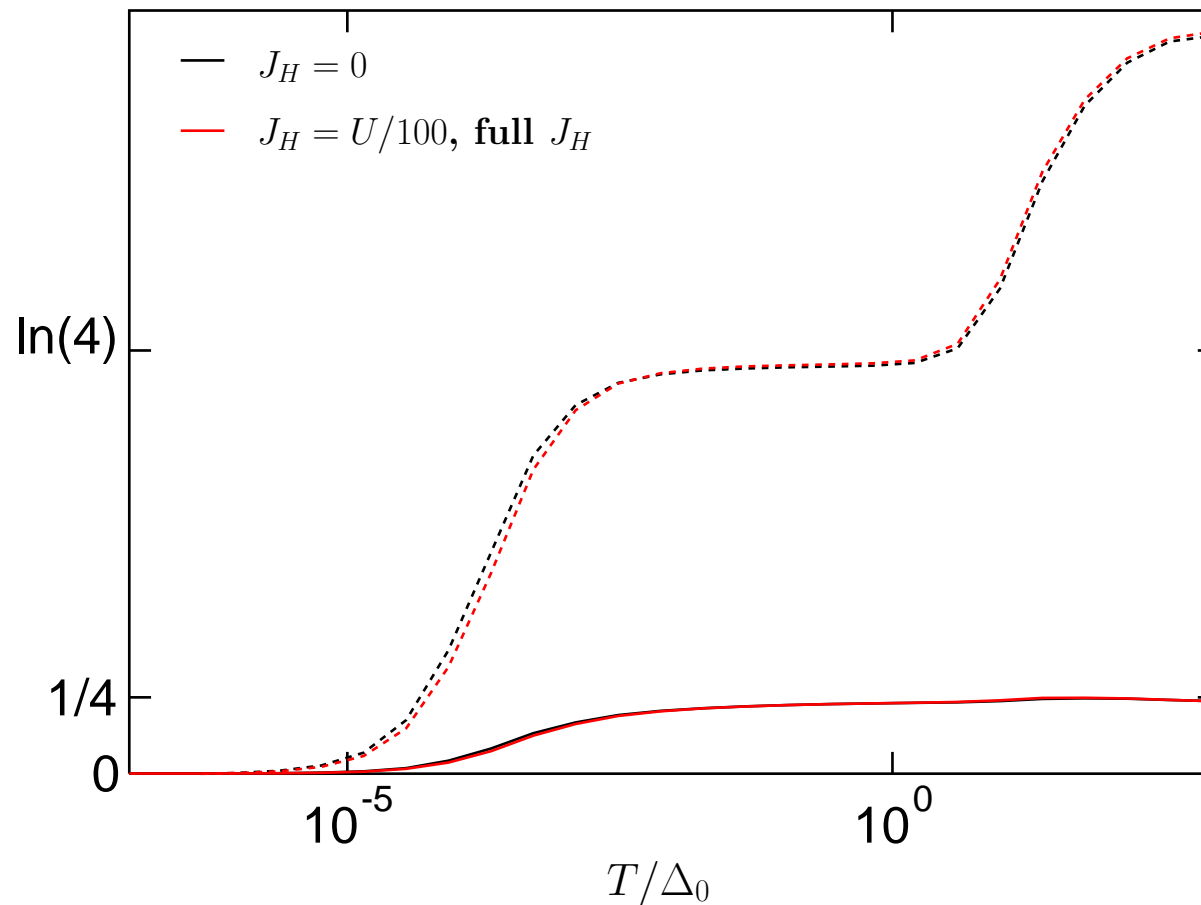


How important is Hund's coupling for $\langle n^d \rangle = 1$?



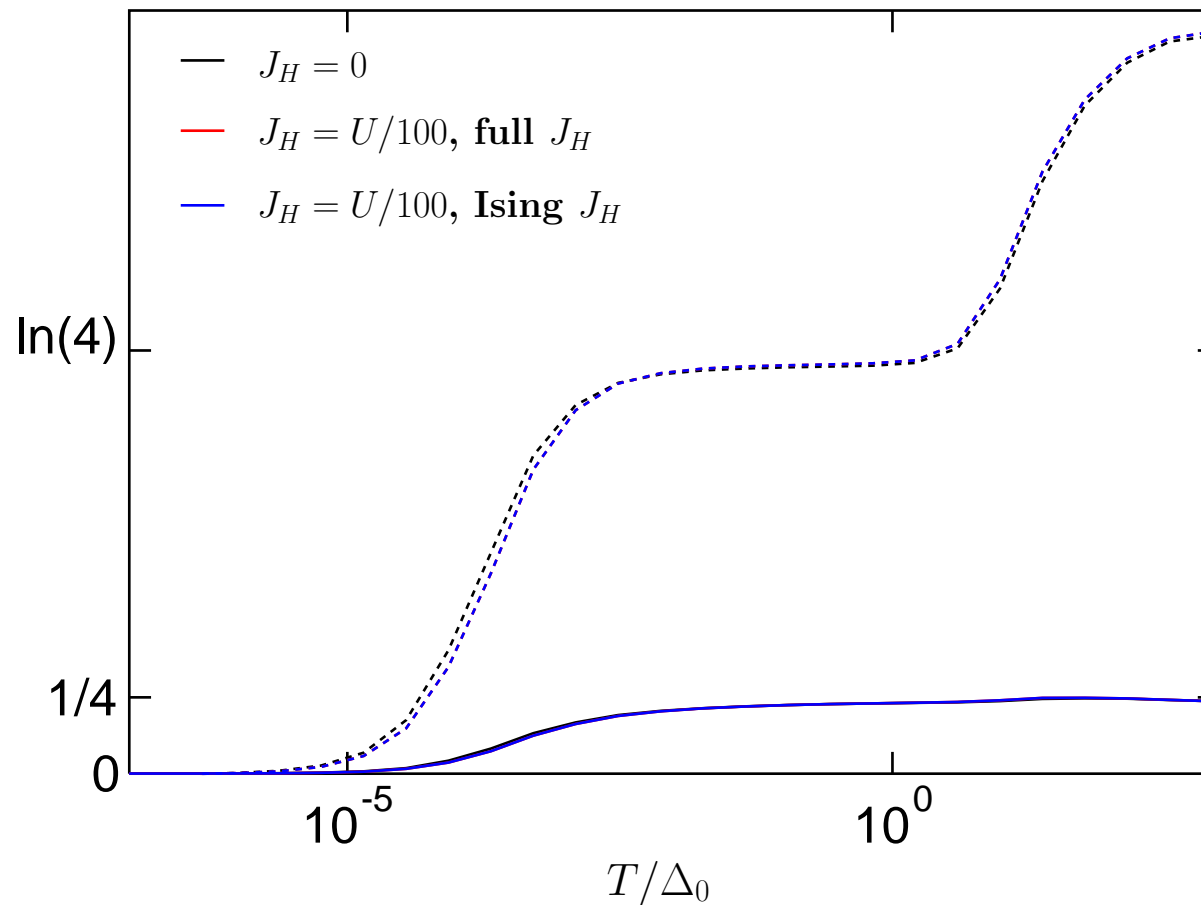


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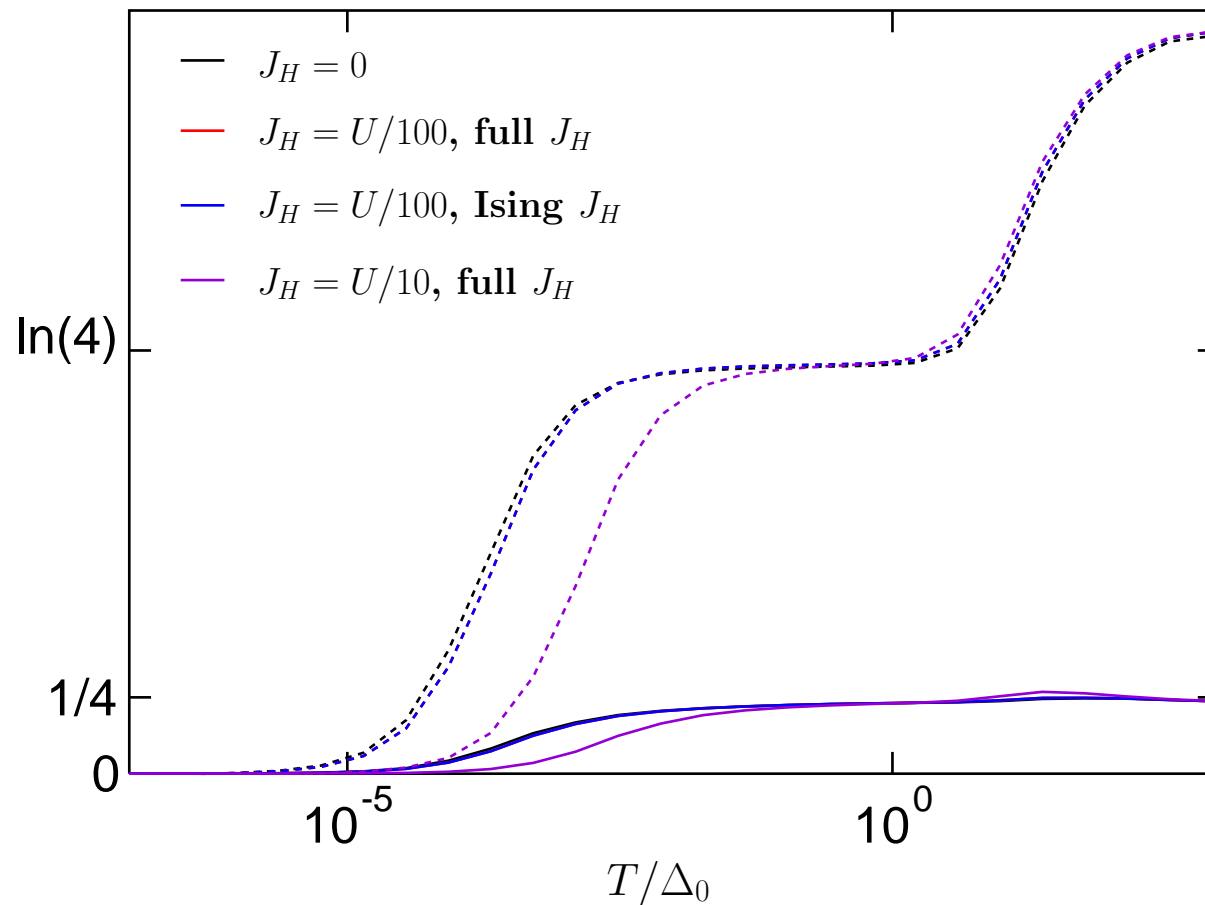


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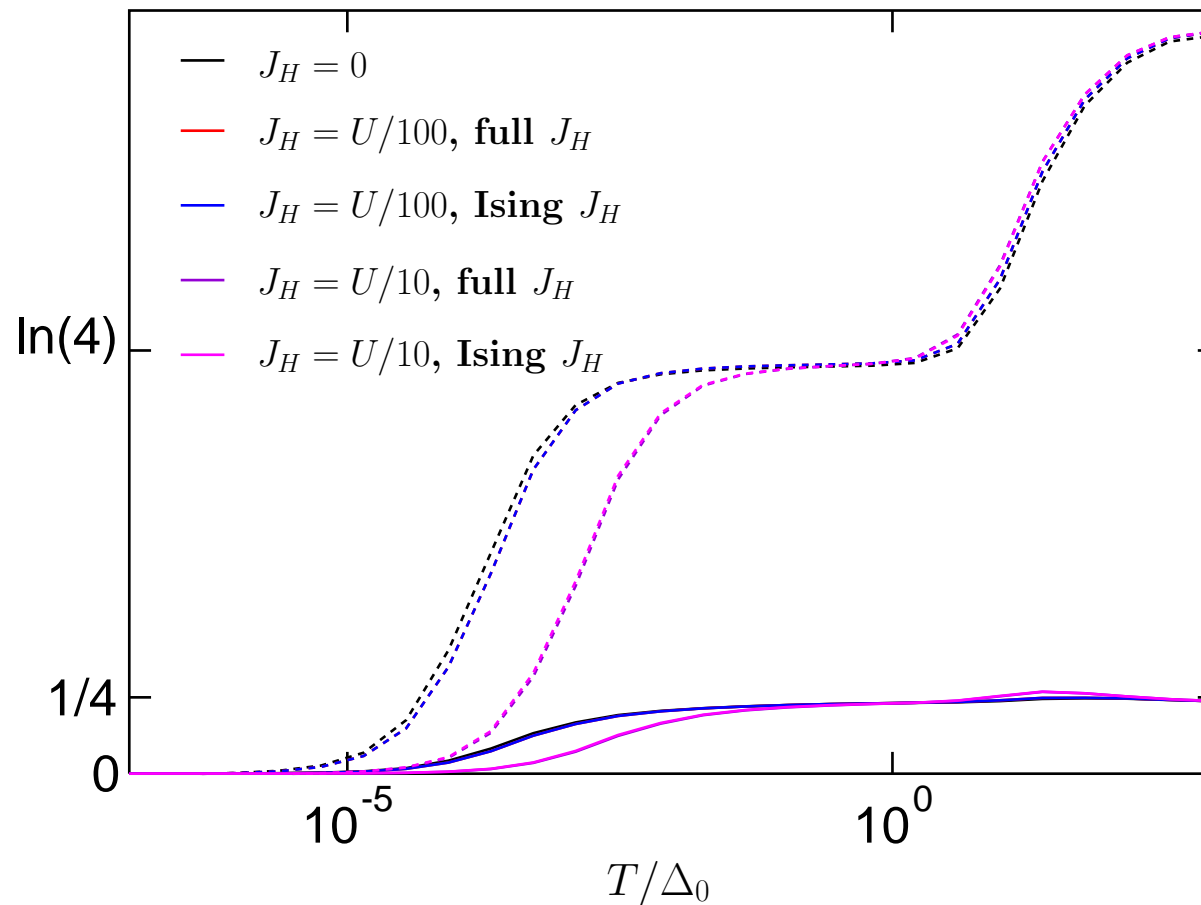


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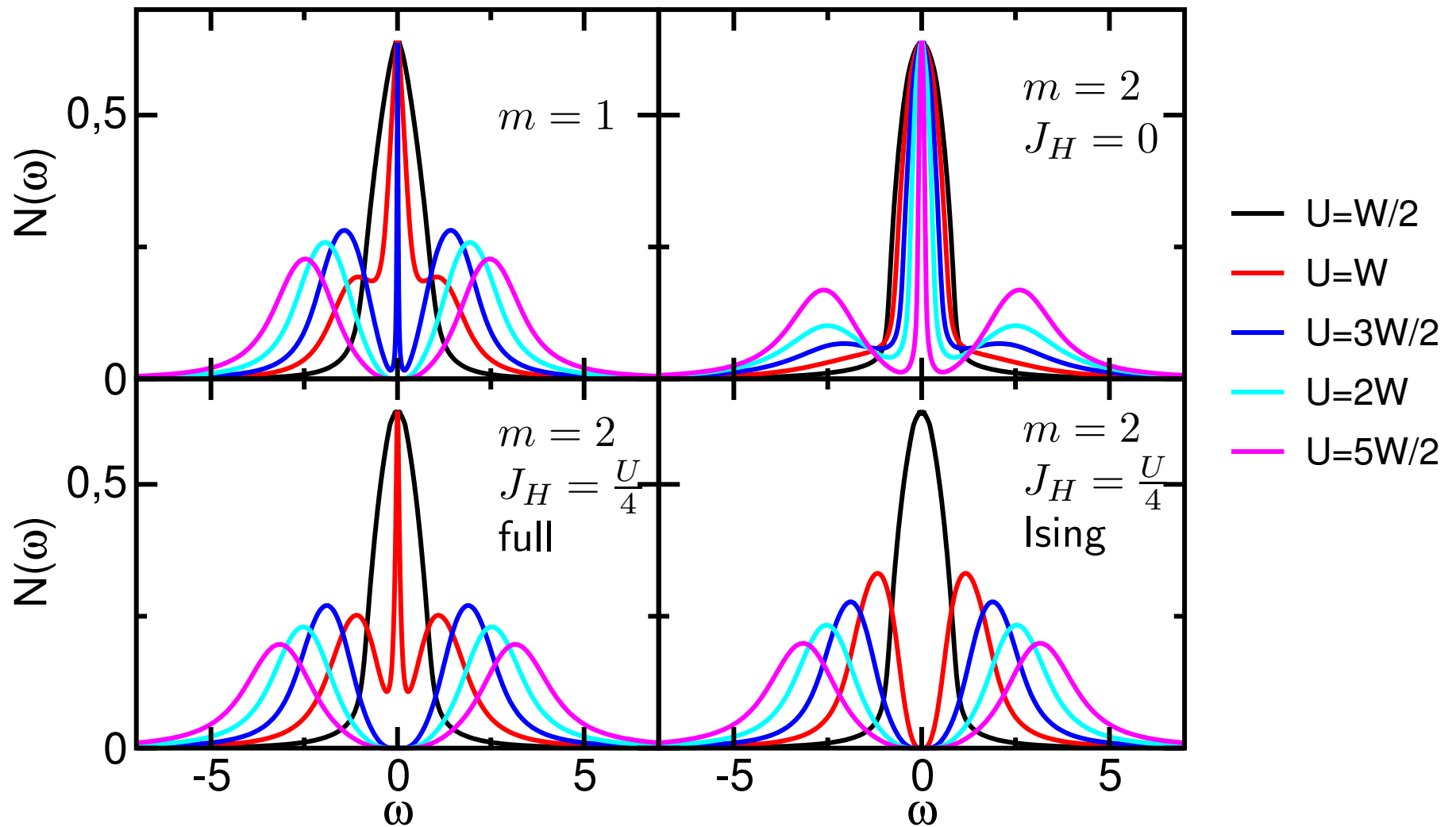
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Mott-Hubbard transition for $\langle n \rangle = 2$ at $T = 0$

(half filling)





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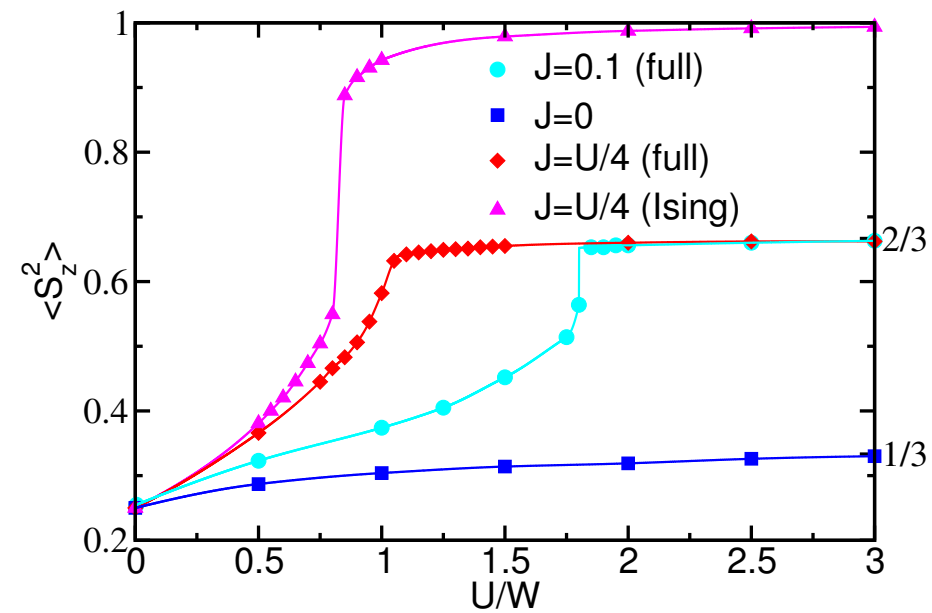
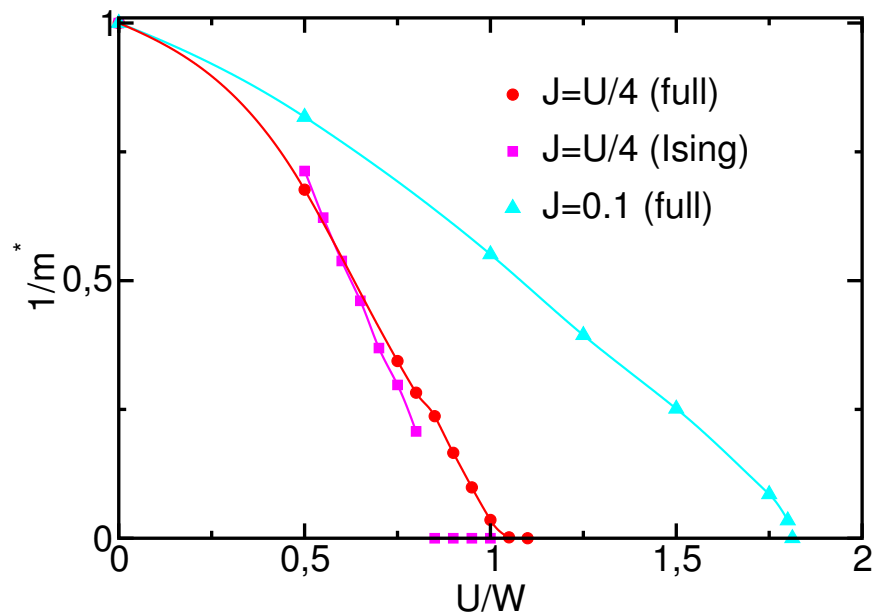
Of what type is the transition at $T = 0$?

(c.f. Ōno et al., PRB ('03))



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- $J = 0$ and full $J = U/4$: Second order

(c.f. $m = 1$)

- $J = \text{const.}$: Possibly weakly first order

(Ōno et al., PRB ('03))

- Ising-like J : Strongly first order



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MIT for filling $\langle n \rangle = 1$

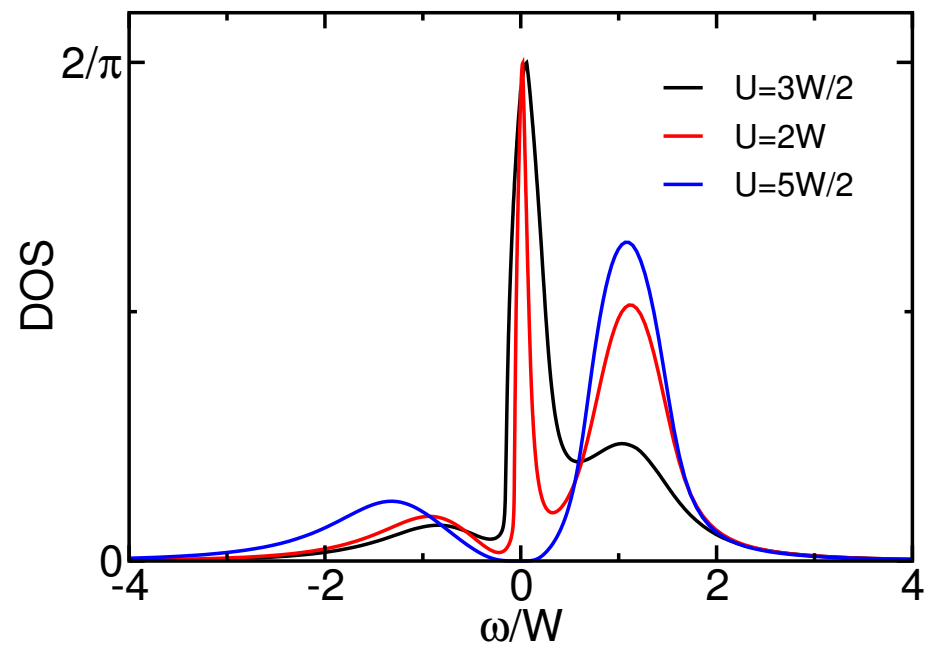
quarter filling



MIT for filling $\langle n \rangle = 1$

quarter filling

$$J_H = 0$$

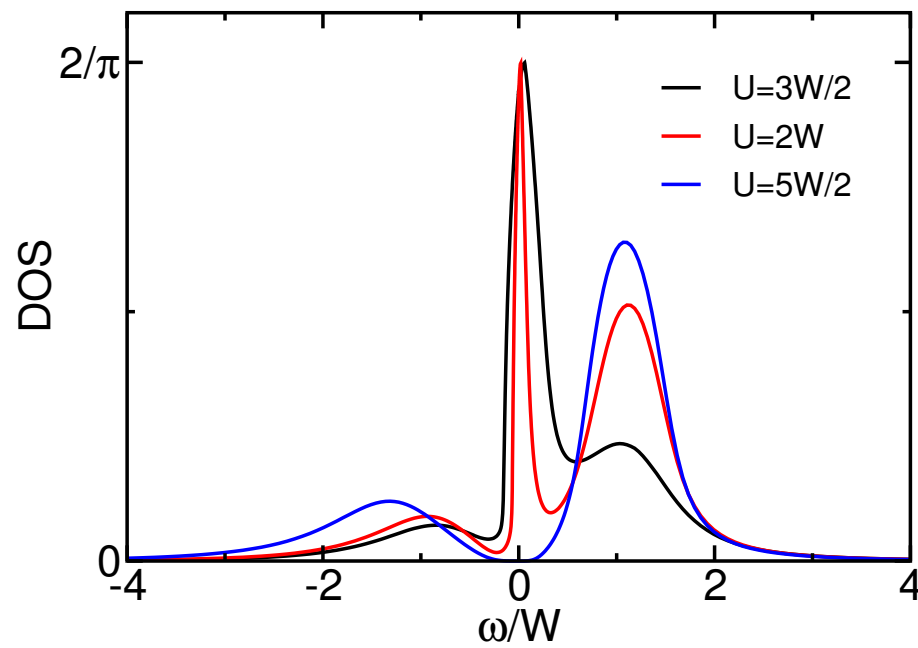




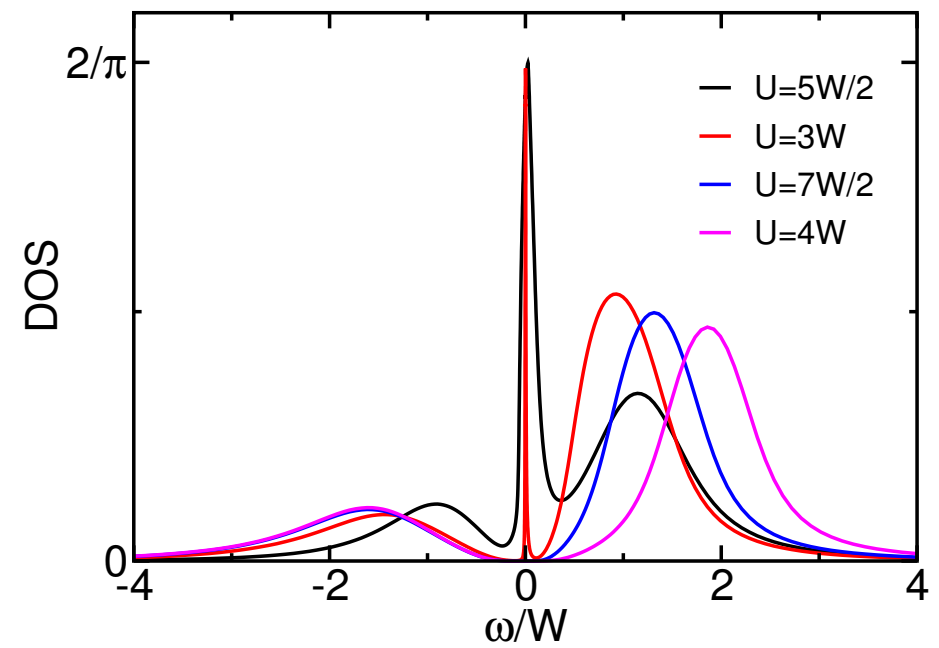
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$$J_H = 0$$



$$J_H = W/4$$





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 - ➡ Hund's coupling vital for low-energy physics
 - ➡ Ising anisotropy: Possible QPT
 - ➡ DMFT: Strongly reduced U_c , nature of MIT



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- Future studies:
 - ➡ Multi-impurity systems
 - ➡ Magnetic and orbital order in TMO