Transport properties of the combined Hubbard - Kondo lattice model

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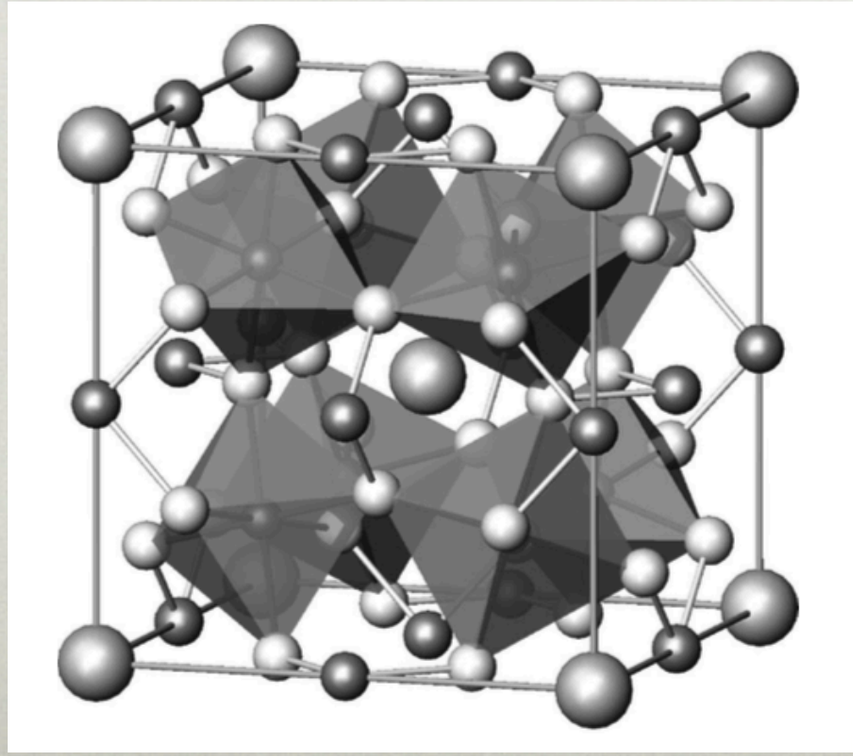
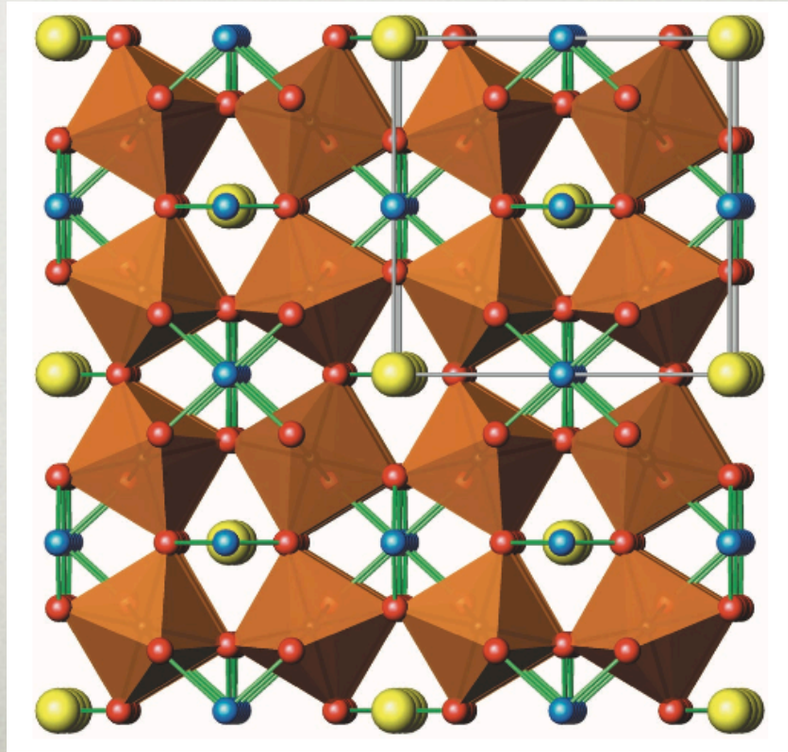
Jožef Stefan institute, Ljubljana, Slovenia

Spin, charge and energy transport in novel materials, Hvar, Oct 2017

quadruple ($AC_3B_4O_{12}$) perovskites

- record high ε in $CaCu_3Ti_4O_{12}$ (ε=10000 in the 100-600K range)
- giant magnetoresistance in $CaCu_3Mn_4O_{12}$
- ferromagnetic isolator $CaCu_3Ge_4O_{12}$
- heavy fermion metal $CaCu_3Ru_4O_{12}$





COPPER RUTHENATES

$ACu_3Ru_4O_{12}$ A=Ca, Na, La,...

Strongly correlated metals:

- moderately enhanced χ and γ γ=290mJ/mol·K^2 for A=Pr
- no magnetic order, Pauli paramagnets
- Kadowaki-Woods relation satisfied
- metallic resistivity, $\varrho_{300\,K}$~1 mΩ cm
- no ϱ saturation, bad metals
- S continuously increases, $S_{900\,K}$~30 μV/K

COPPER RUTHENATES

bad metals due to U & J ?

heavy fermions due to Kondo-like physics?

Where is the spin?

a) $3d^9$ Cu^{2+} S=½ magnetic cations, itinerant Ru *d* electrons

b) scattering of conduction electrons on $4d^4$ Ru^{4+} S=1 sites

Kobayashi et al., J. Phys. Soc. Jpn. **73**, 2373 (2004)
Xiang, Liu, Zhao, Meng, Wu, Phys. Rev. B **76**, 155103 (2007)
Tanaka, Shimazui, Takatsu, Yonezawa, Maeno, J. Phys. Soc. Jpn. **78**, 024706 (2009)
Krimmel, Phys. Rev. B **80**, 121101(R) (2009)
Hollmann et al., Phys. Rev. B **87**, 155122 (2013)
Hébert, Daou, Maignan, Phys. Rev. B **91**, 045106 (2015)
Günther, PhD thesis, Uni. Augsburg (2015)
Riegg et al., Phys Rev. B **93**, 115149 (2016)
Kao et al., Phys. Rev. B **96**, 024402 (2017)

Another related system: $Nd_{2-x}Ce_xCuO_4$

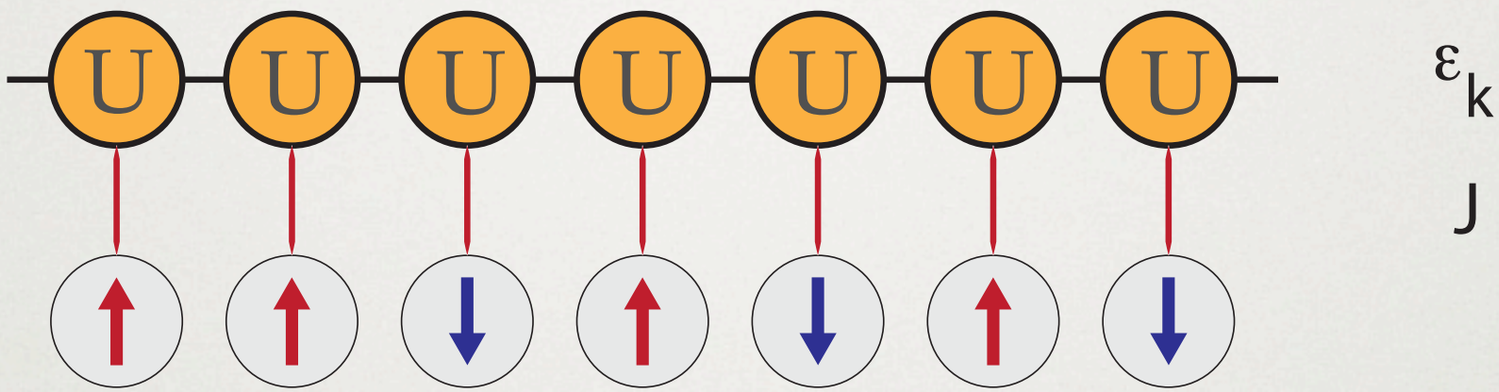
For T<0.3K, linear specific heat, $\gamma \simeq 4$ J/(mol K^2),
χ constant, Sommerfeld-Wilson ratio of order 1.

Unexpectedly low $T_{coh} \sim 1K$.

Undoped Nd_2CuO_4 is AFM charge-transfer insulator, i.e., a strongly correlated system.

Schork, Fulde, PRB **50**, 1345 (1994)
Igarashi, Muruyama, Fulde, PRB **52**, 15966 (1995)
Schork, Blawid, PRB **56**, 6559 (1997)
Hagymósi, Itai, Sólyom, PRB **85**, 235116 (2012)

COMBINED HUBBARD - KONDO LATTICE MODEL



$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + J \sum_i \mathbf{s}_i \cdot \mathbf{S}_i$$

Hubbard model + one spin on each lattice site

equivalently: KLM with interacting conduction electrons

Shibata, Nishino, Ueda, Ishii, PRB **53**, 8828 (1996)
Itai, Fazekas, PRB **54**, 752(R) (1996)
Schork, Blawid, Igarashi, PRB **59**, 9888 (1999)
Peters, Pruschke, PRB **76**, 245101 (2007)
Yoshida, Ohashi, Kawakami, JPSJ **80**, 063710 (2011)

- DMFT(NRG) at high temperatures
- Limiting cases: pure HM, pure KLM
- Characteristic temperature scales in combined HM+KLM
- High-T asymptotics: do spins decouple?
- Thermopower in combined model

Conductivity for d=∞

No vertex corrections, just "zero-th order bubble":

$$\sigma = 2\pi D \sigma_0 \int d\omega \int d\epsilon \left(-\frac{\partial f}{\partial \omega}\right) \phi(\epsilon) A^2(\epsilon, \omega)$$

$$\sigma_0 = e^2 \hbar \Phi(0)/D$$ Mott-Ioffe-Regel conductivity

$$\Phi(\epsilon) = \sum_{\mathbf{k}} \left(\frac{\mathrm{d}\epsilon_{\mathbf{k}}}{\mathrm{d}k_x}\right)^2 \delta(\epsilon - \epsilon_{\mathbf{k}}) \qquad \phi(\epsilon) = \Phi(\epsilon)/\Phi(0)$$

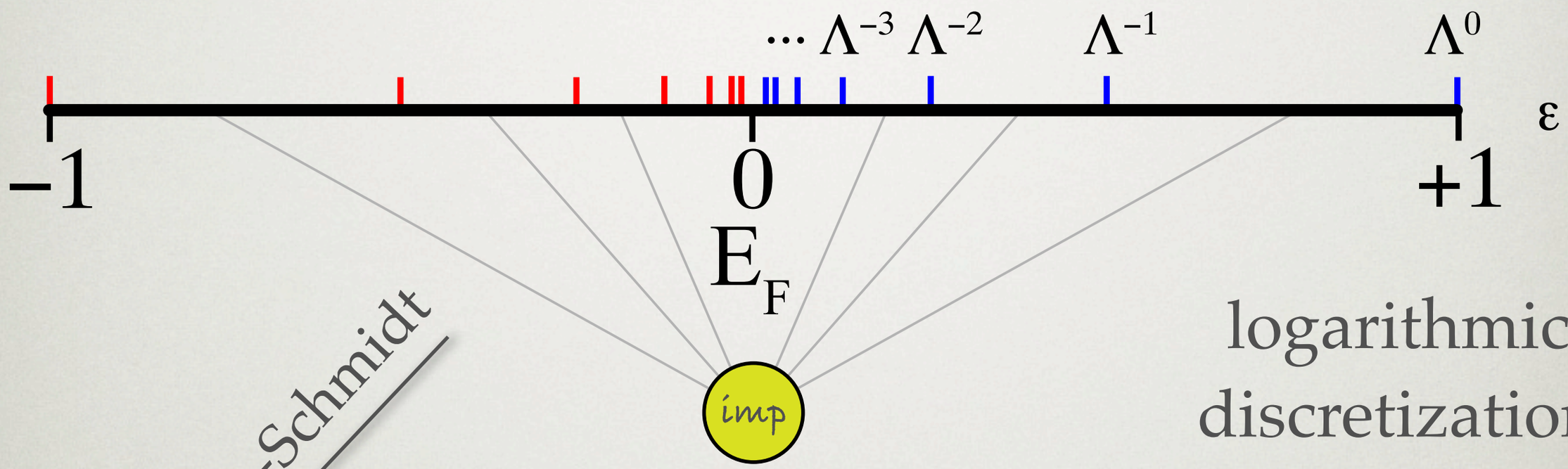
$$A(\epsilon, \omega) = \frac{1}{\omega - \epsilon - \Sigma(\omega)}$$

computed within the dynamical mean-field theory (DMFT) approach

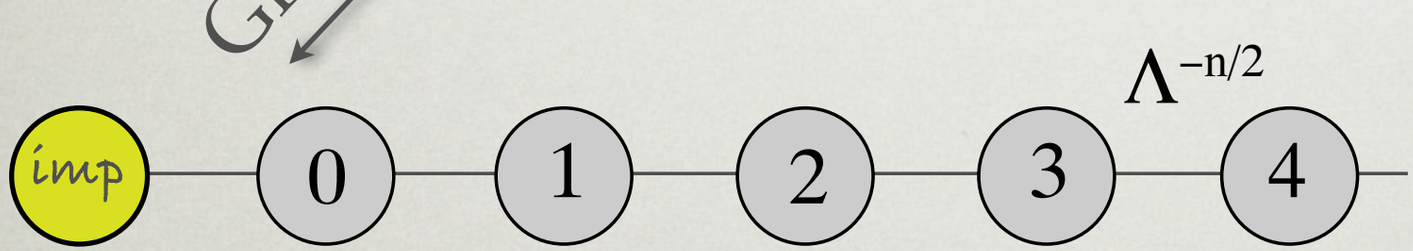
Metzner, Vollhardt, PRL **62**, 324 (1989)
Georges, Kotliar, Krauth, Rozenberg, RMP **68**, 13 (2006)
Khurana, PRL **64**, 1990 (1990)

Numerical Renormalization Group

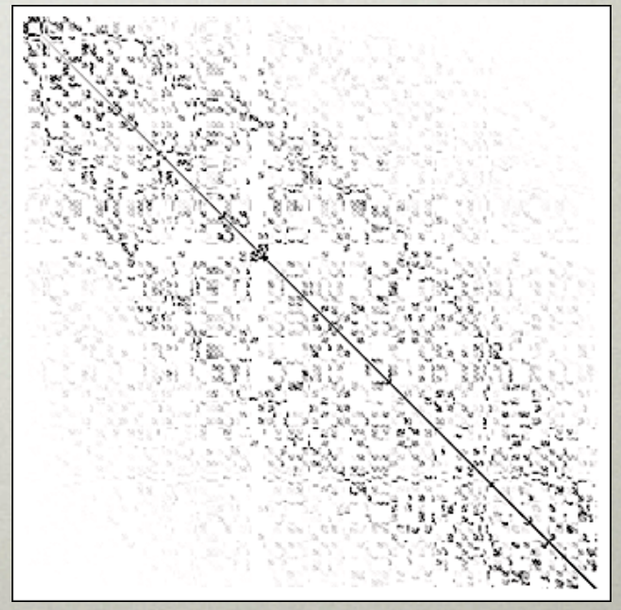
K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975)



logarithmic discretization $\Lambda>1$



Wilson's chain



http://nrgljubljana.ijs.si/

Artifact-less discretization schemes for the NRG

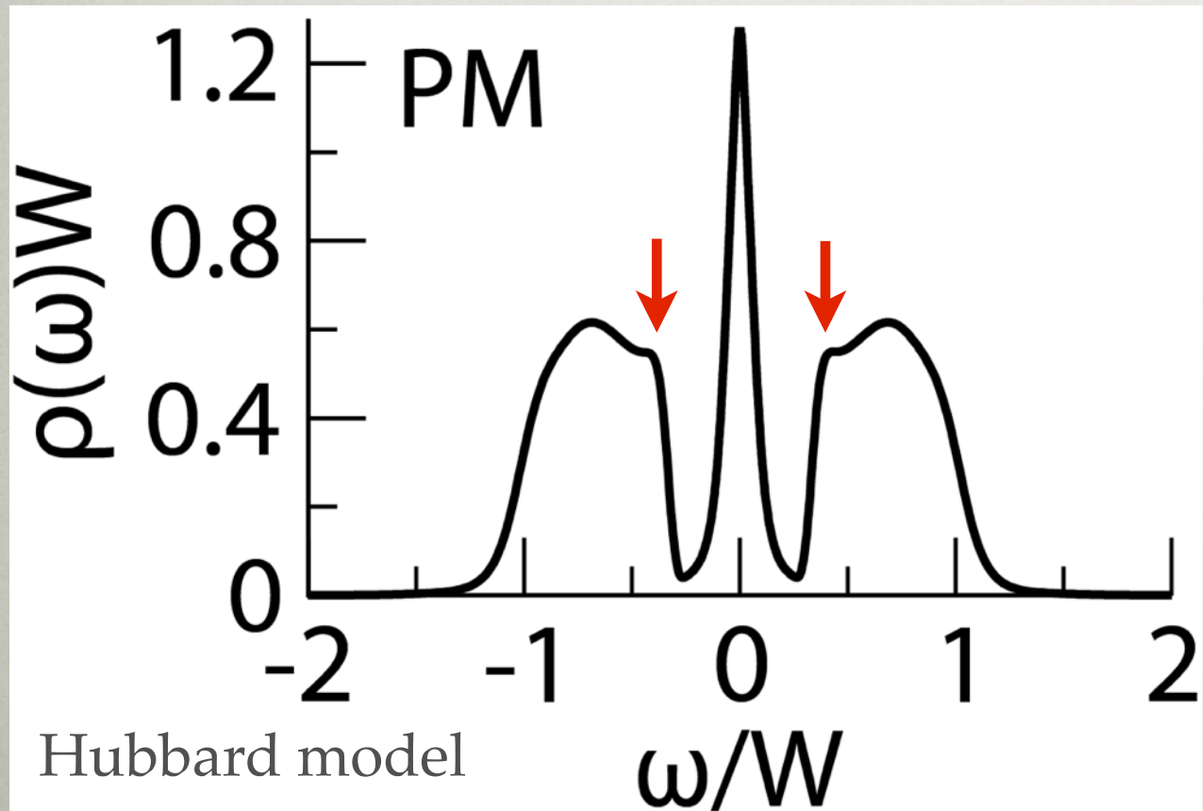
$$A_{f_0}(\omega) = \rho(\omega)$$

$$\frac{\int_{I_j} \rho(\epsilon)\,\mathrm{d}\epsilon}{|\mathrm{d}\mathcal{E}_j^z/\mathrm{d}z|} = \rho(\omega)$$

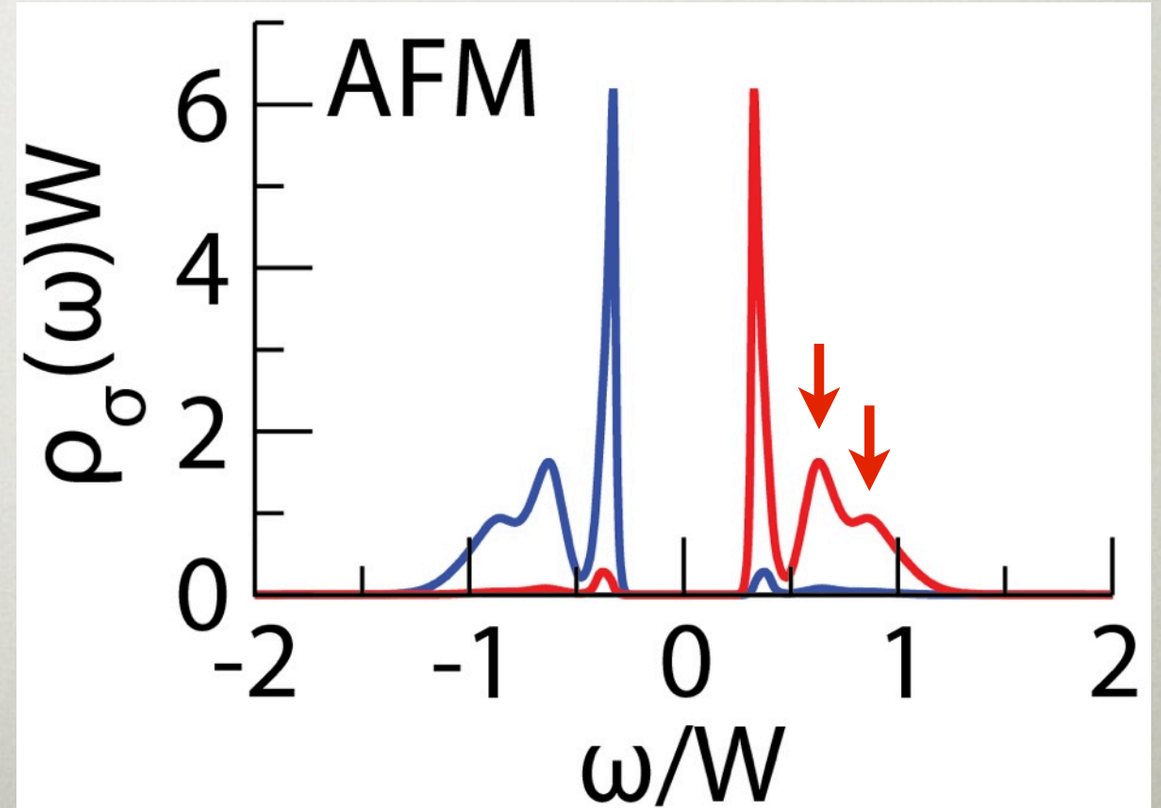
$$\mathcal{E}(x) = Df(x)\Lambda^{2-x} \qquad x = j + z$$

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} = \ln\Lambda\, f(x) - \frac{\int_{\epsilon(x+1)}^{\epsilon(x)} \rho(\omega)\,\mathrm{d}\omega}{\Lambda^{2-x}\rho[\mathcal{E}(x)]}$$

R. Žitko, Th. Pruschke, PRB **79**, 085106 (2009)
R. Žitko, Comput. Phys. Comm. **180**, 1271 (2009)



Hubbard model

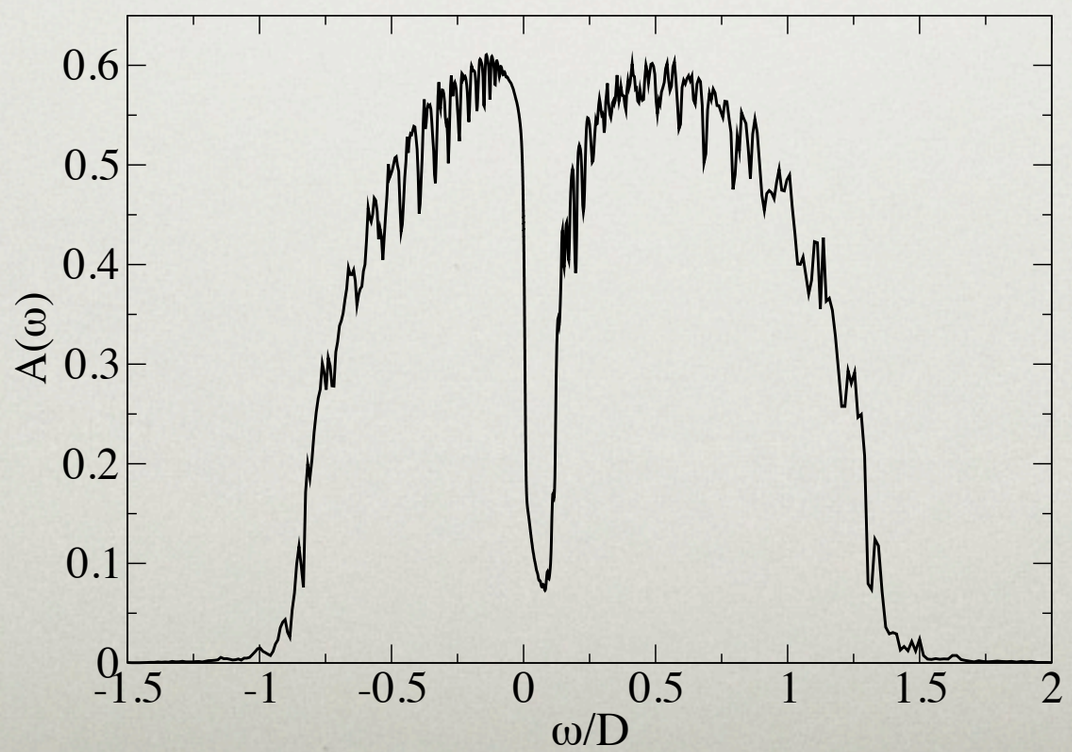


NRG in the limit of very high temperatures

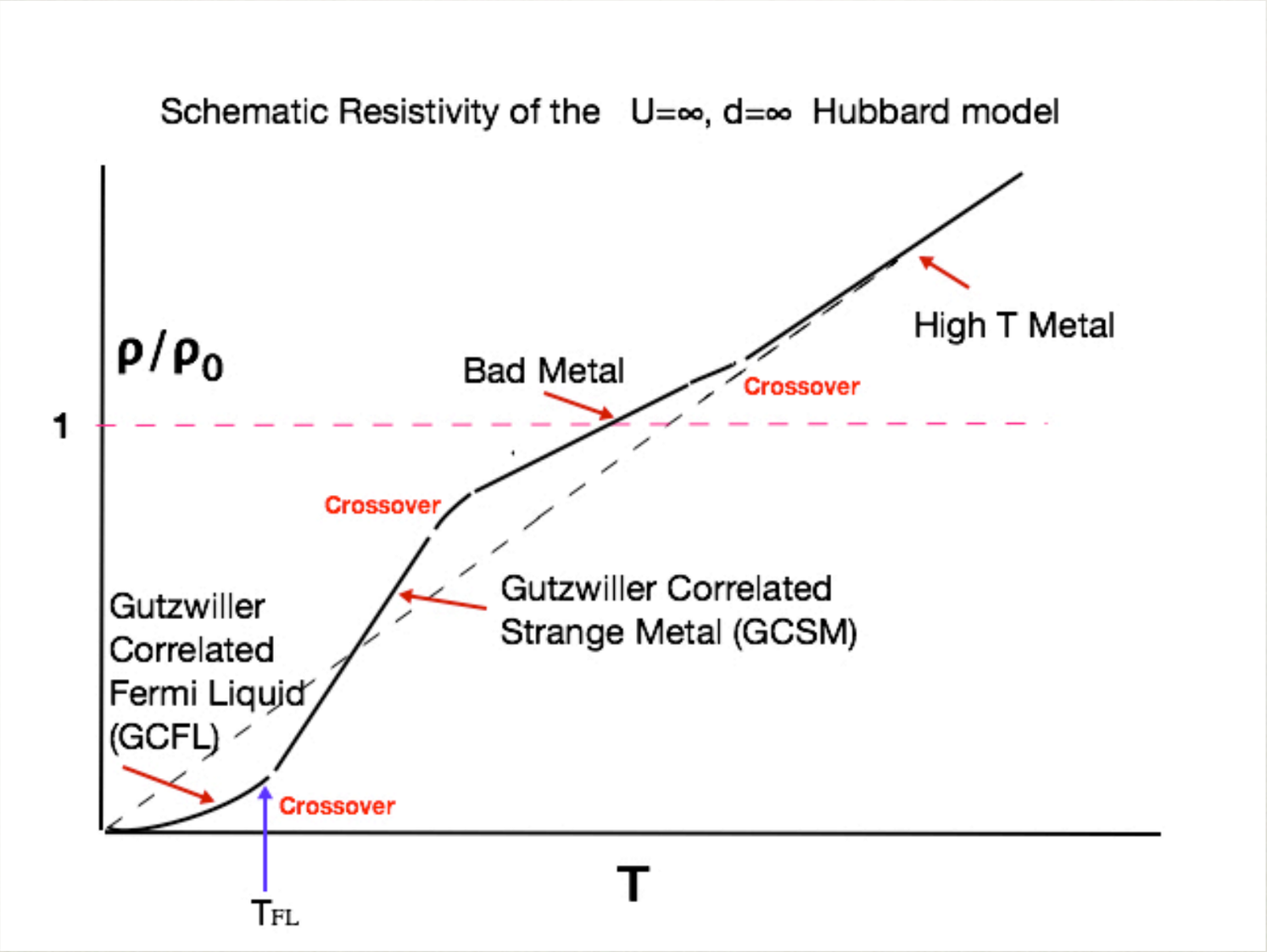
Turns out, it works!

<u>Recipe</u>:

- Gaussian broadening with constant kernel width w
- reduce w until integrated quantities are converged (overbroadening → overestimated ϱ)



Transport in pure Hubbard model

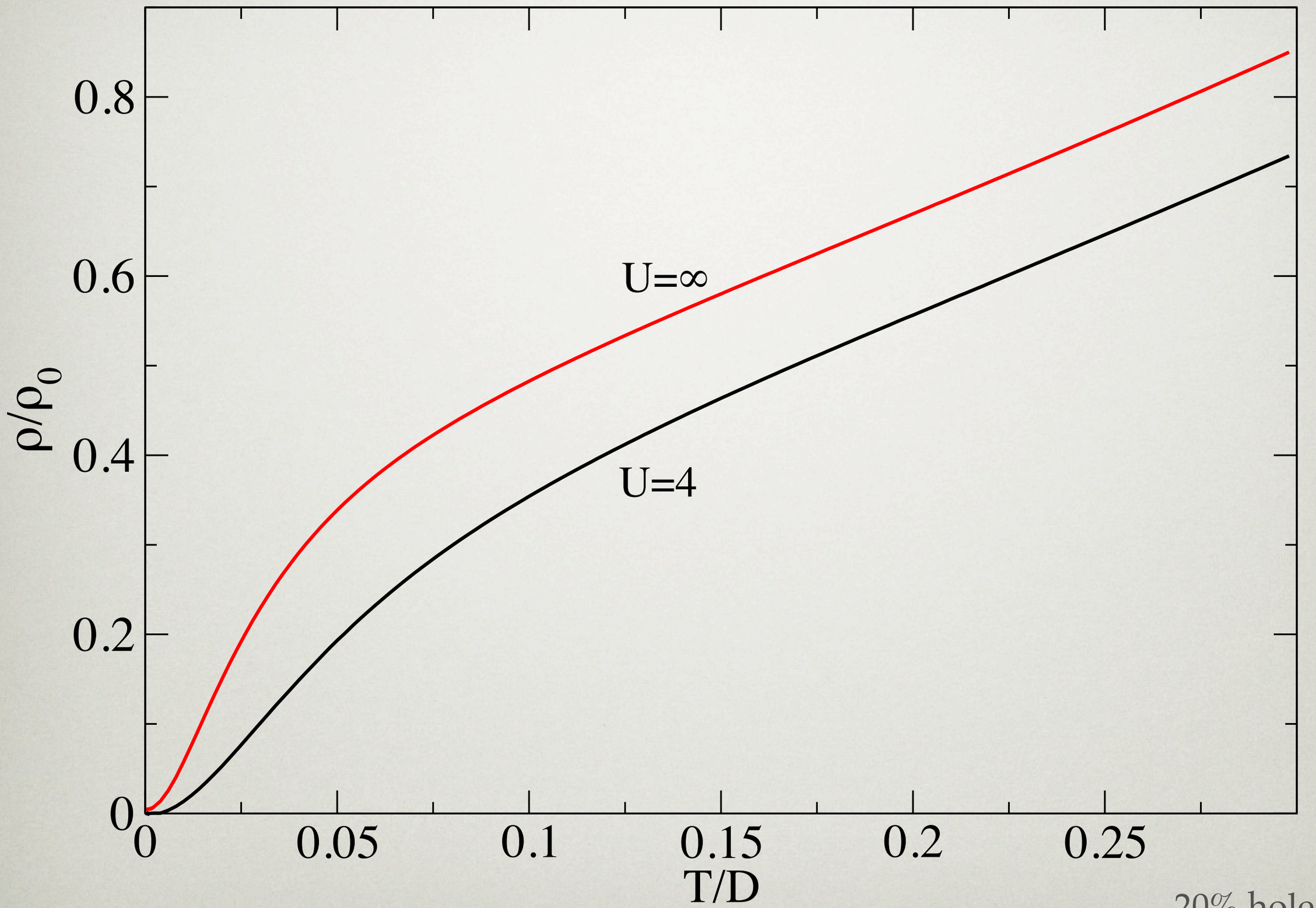


Deng et al., PRL **110**, 086401 (2013)
Žitko et al., PRB **88**, 235132 (2013)
Perepelitsky et al., PRB **94**, 235115 (2016)
Ding et al., PRB **96**, 054114 (2017); Ding et al., PRB **96**, 115153 (2017)

Talks by Sriram Shastry and Edward Perepelitsky

ρ_0 = Mott-Ioffe-Regel resistivity

D = half-bandwidth (also used as the energy unit)

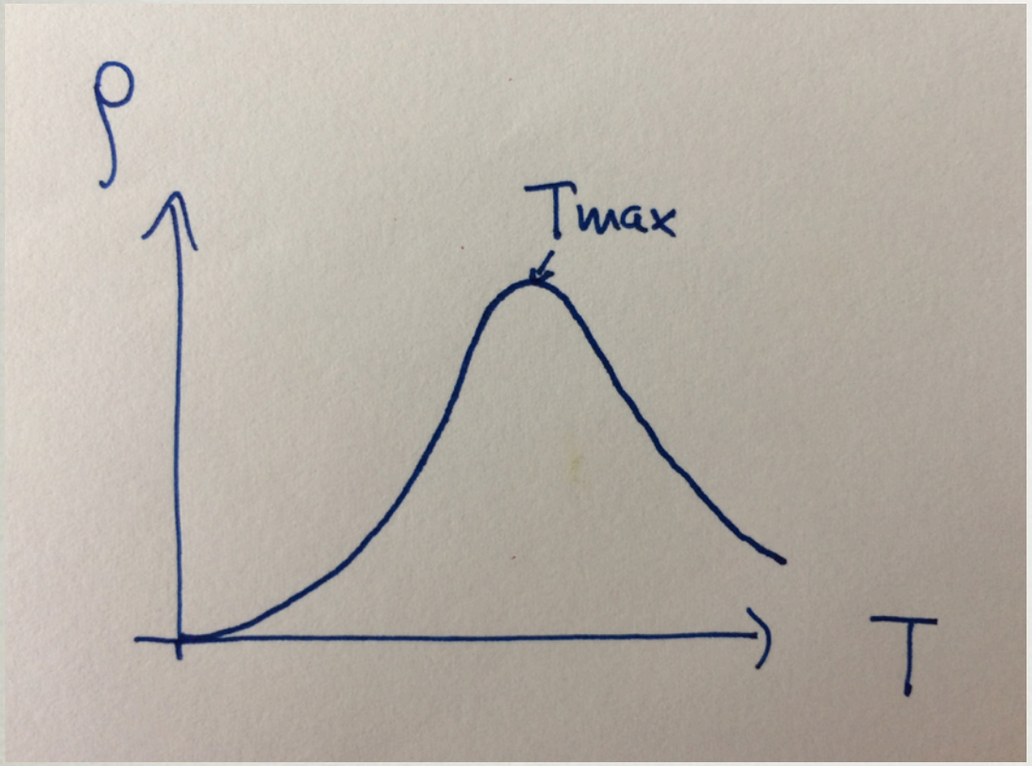


20% hole doping

n=0.8

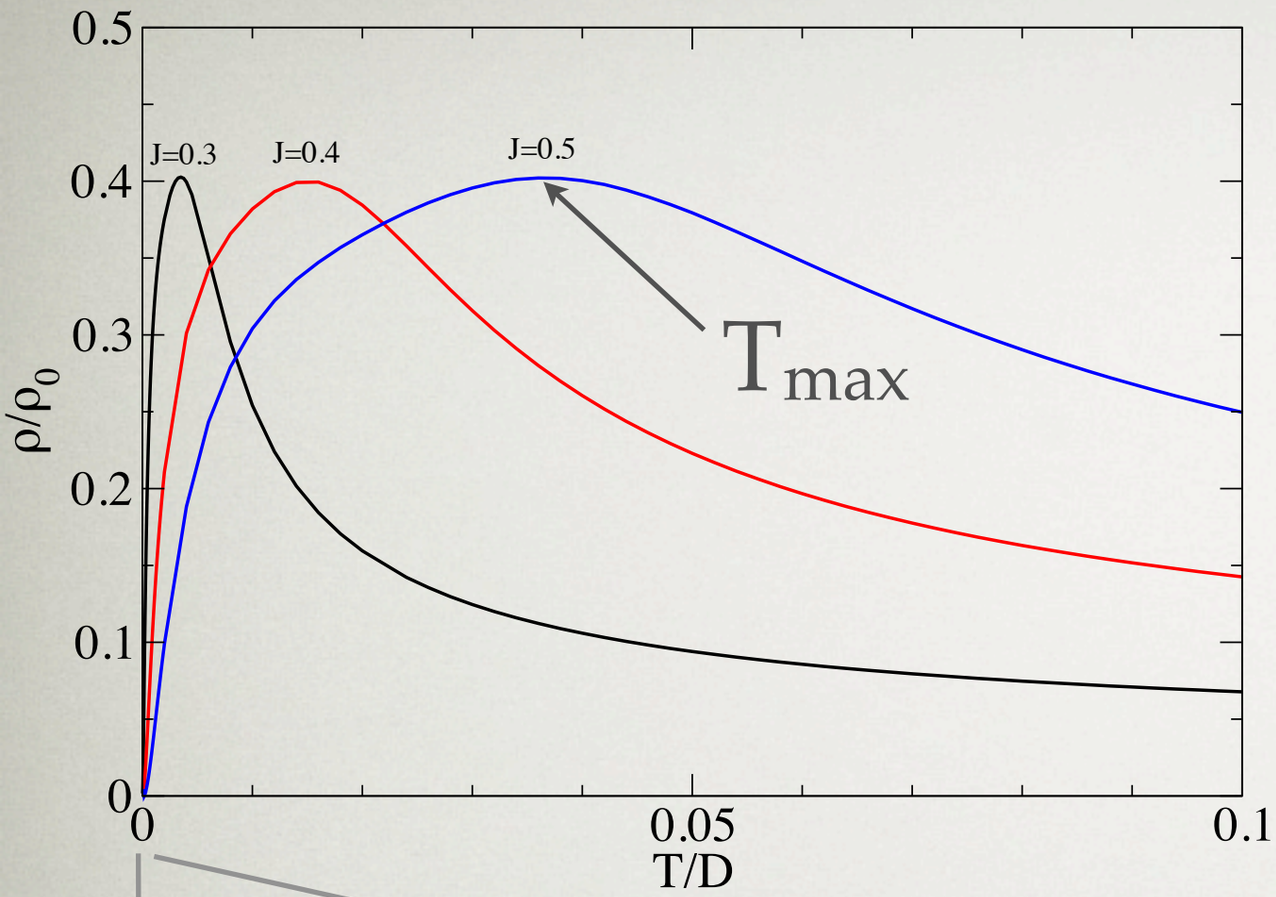
DMFT(NRG) calculation

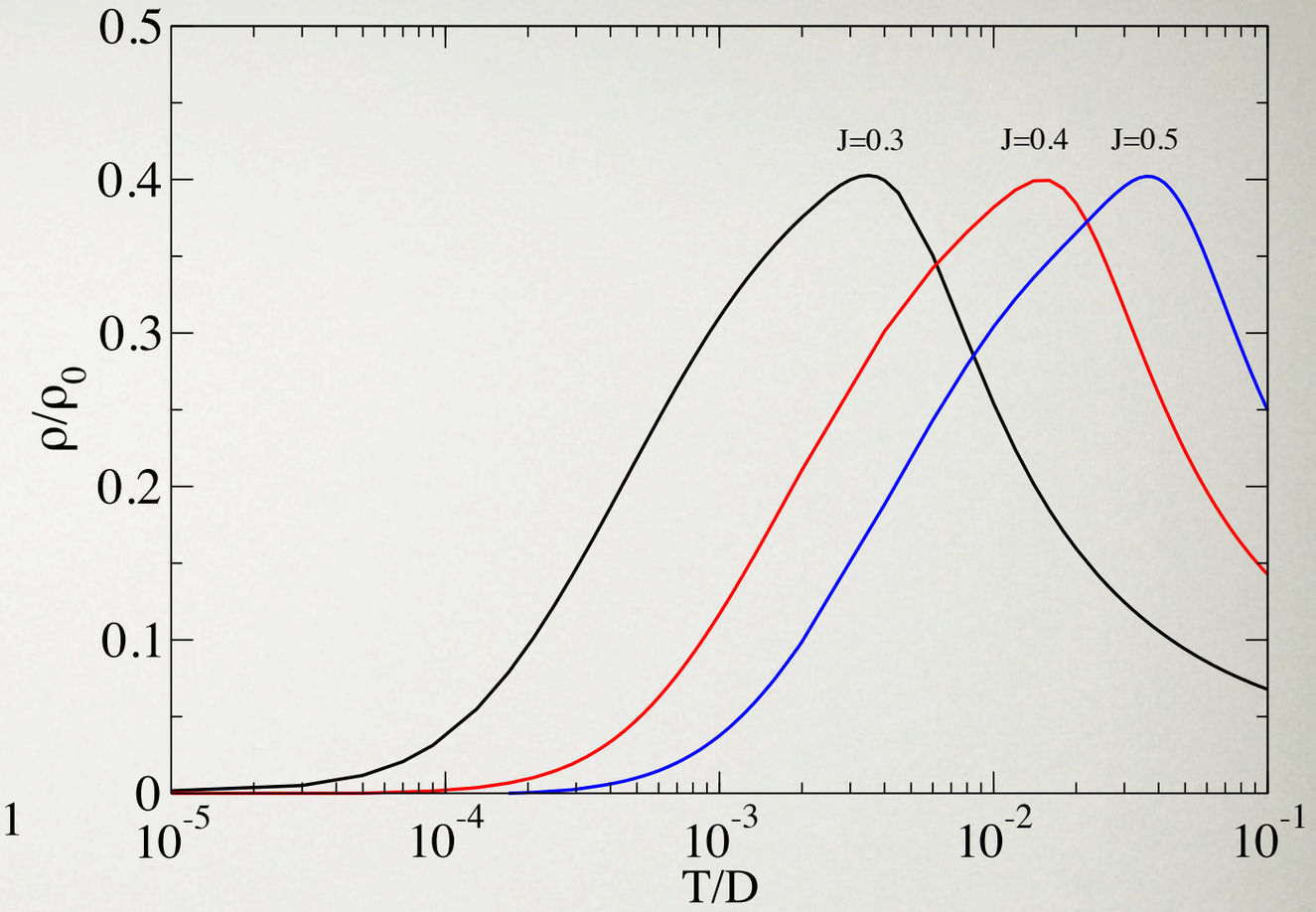
Transport in pure Kondo lattice model

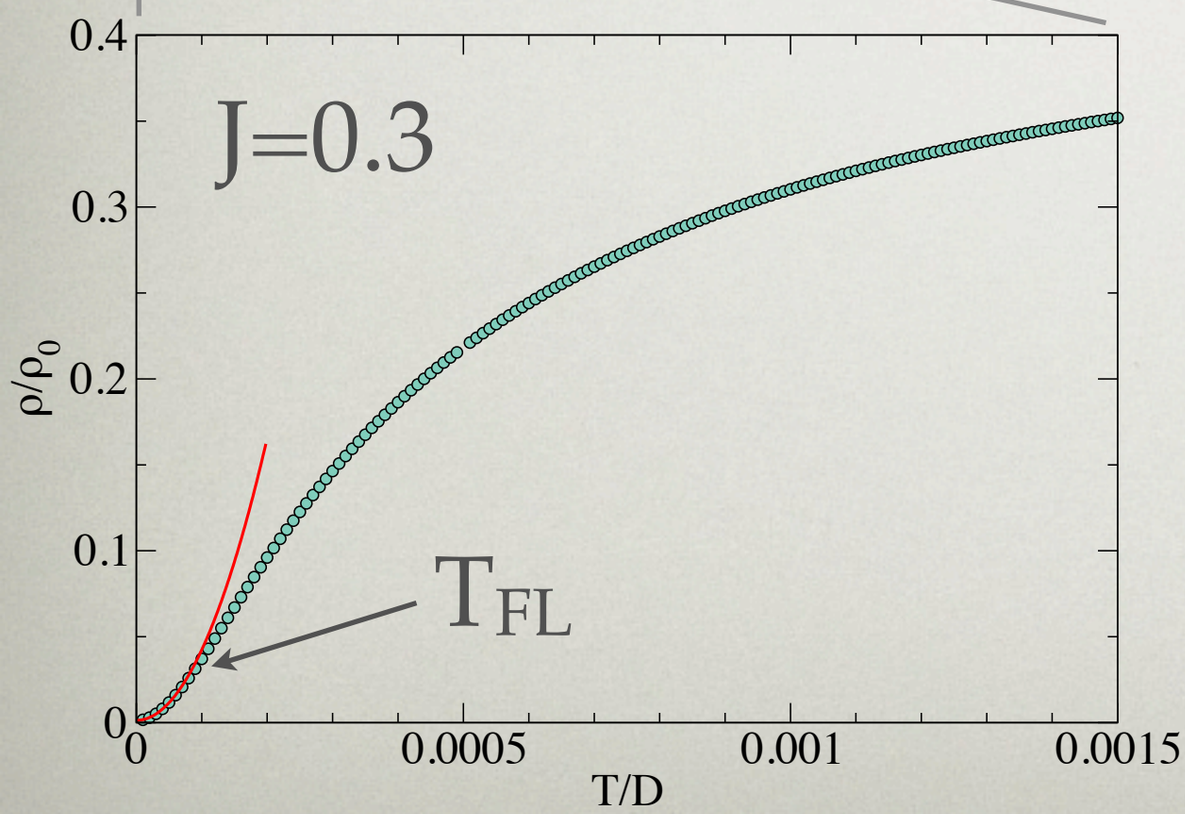


- How many low-energy scales?
- Dependence on exchange coupling J and carrier density n?

Burdin, Georges, Grempel: PRL **85**, 1048 (2000)
Costi, Manini, JLTP **126**, 835 (2002)
Pruschke, Bulla, Jarrell, PRB **61**, 12799 (2000)
Burdin, Zlatić: PRB **79**, 115139 (2009)
S. Burdin: Proceedings of the NATO ARW of Hvar (2008)
Grenzenbach, Anders, Czycholl, Pruschke, PRB **74**, 195119 (2006)
Tahvildar-Zadeh, Jarrell, Freericks: PRB **55**, R3332 (1997)
Vidyadhiraja, Smith, Logan, Krishnamurthy, JPCM **15**, 4045 (2003)





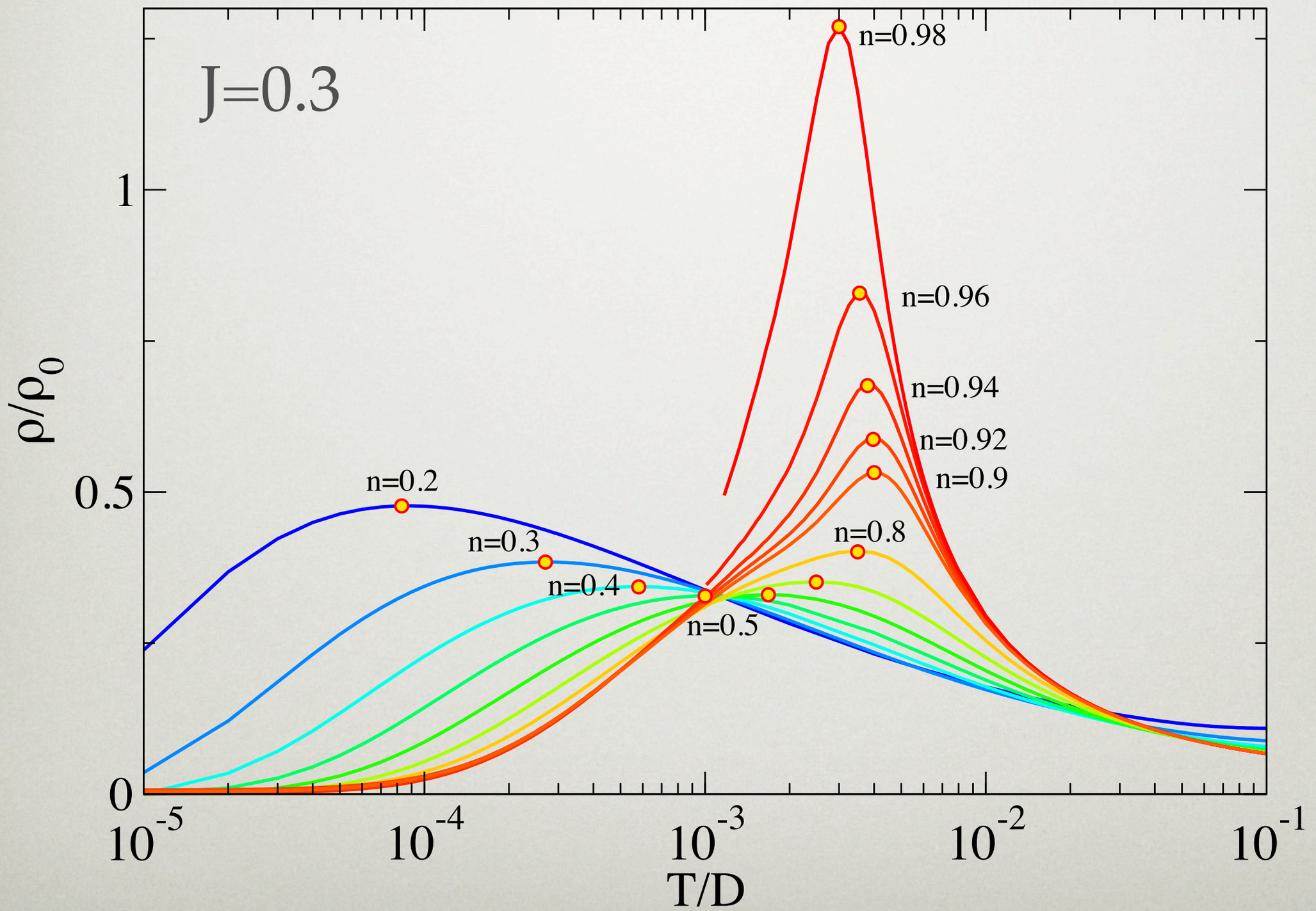


$T_{FL} << T_{max}$

n=0.8

DMFT(NRG) calculation

Doping dependence



Band-correlation effects on single impurities

Kondo model → T_K enhanced

U helps Kondo singlet formation because more strongly correlated electron gas offers more uncompensated spins (enhancement of local spin susceptibility by U).

Anderson impurity model → T_K non-monotonic

grows for small U,
decreases for large U

Large U blocks hybridization, decreases the effective Kondo coupling J.

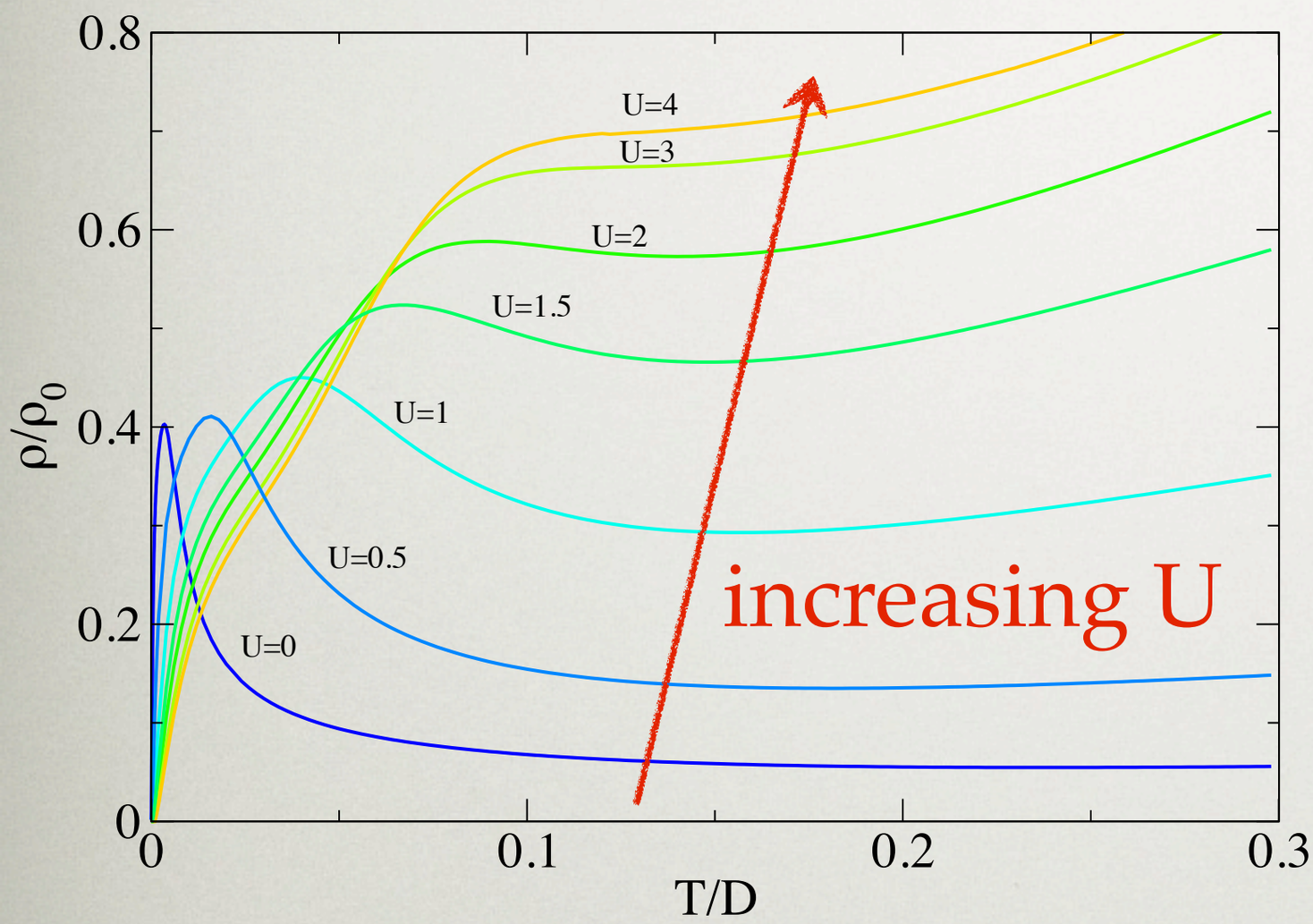
$$J = \frac{8V^2}{U_c + U_f}$$

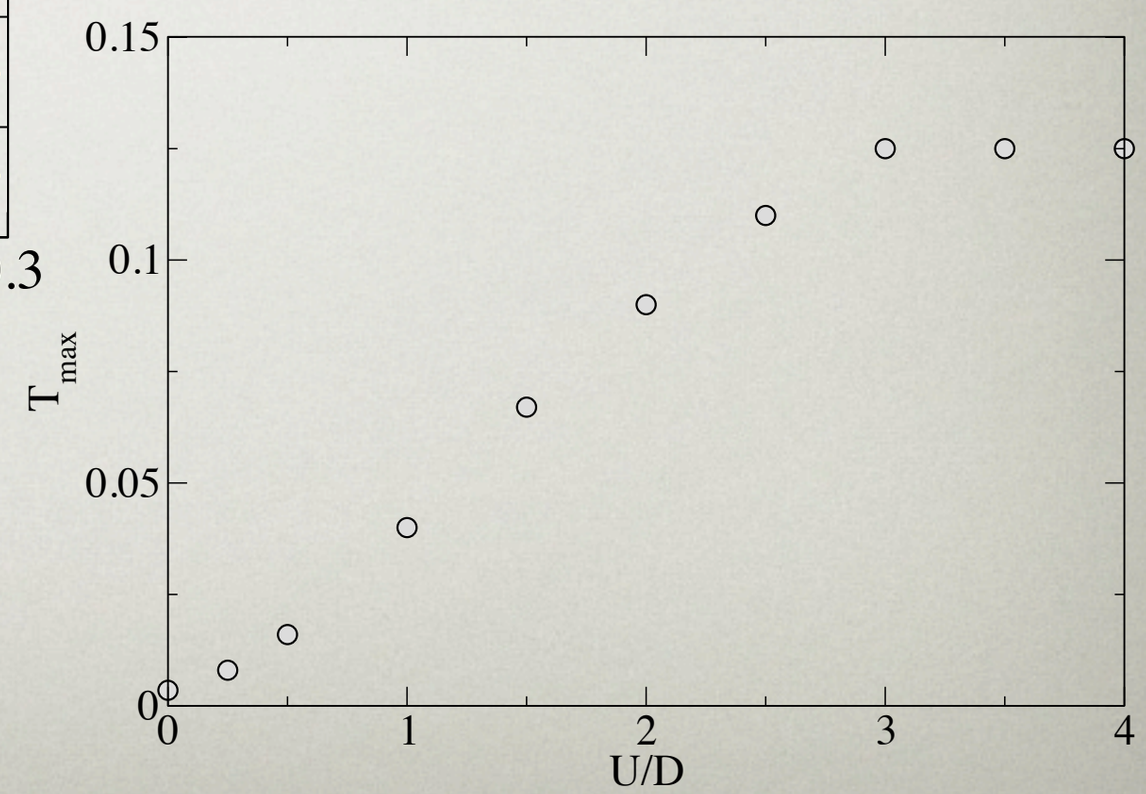
Schork, Fulde, PRB **50**, 1345 (1994)
Li, PRB **52**, R6979 (2005)
Khaliullin, Fulde, PRB **52**, 9514 (1995)
Shibata, Nishino, Ueda, Ishii, PRB **53**, R8828 (1996)
Itai, Fazekas, PRB **54**, R752 (1996)

Schork, PRB **53**, 5626 (1996)
Schiller, Ingersent, Europhys. Lett. **39**, 645 (1997)
Hofstetter, Bulla, Vollhardt, PRL **84**, 4417 (2000)
Neef, Tornow, Zevin, Zwicknagl, PRB **68**, 035114 (2003)
Nishimoto, Fulde, PRB **76**, 035112 (2007)

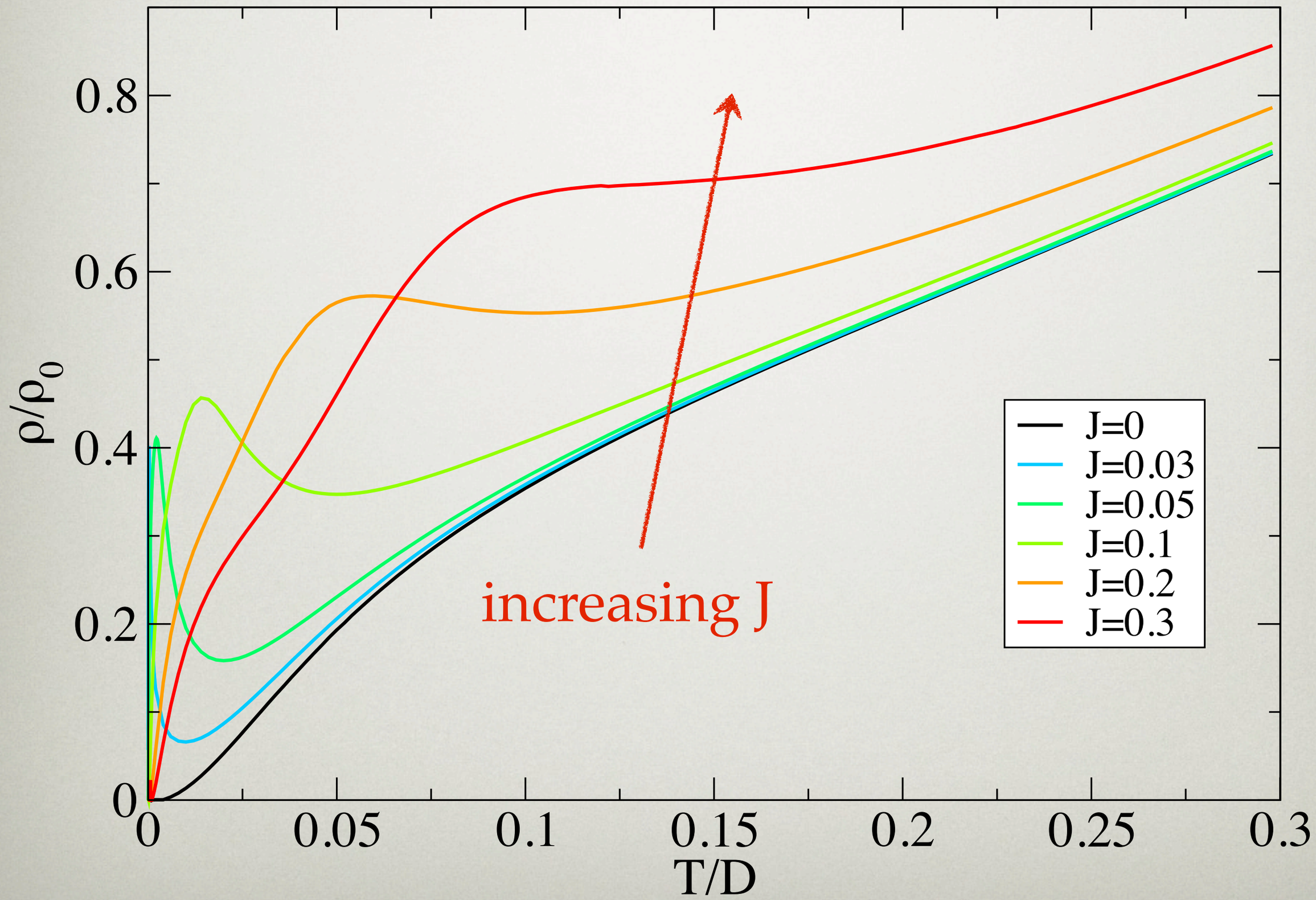
Combined HM+KLM

J=0.3, n=0.8

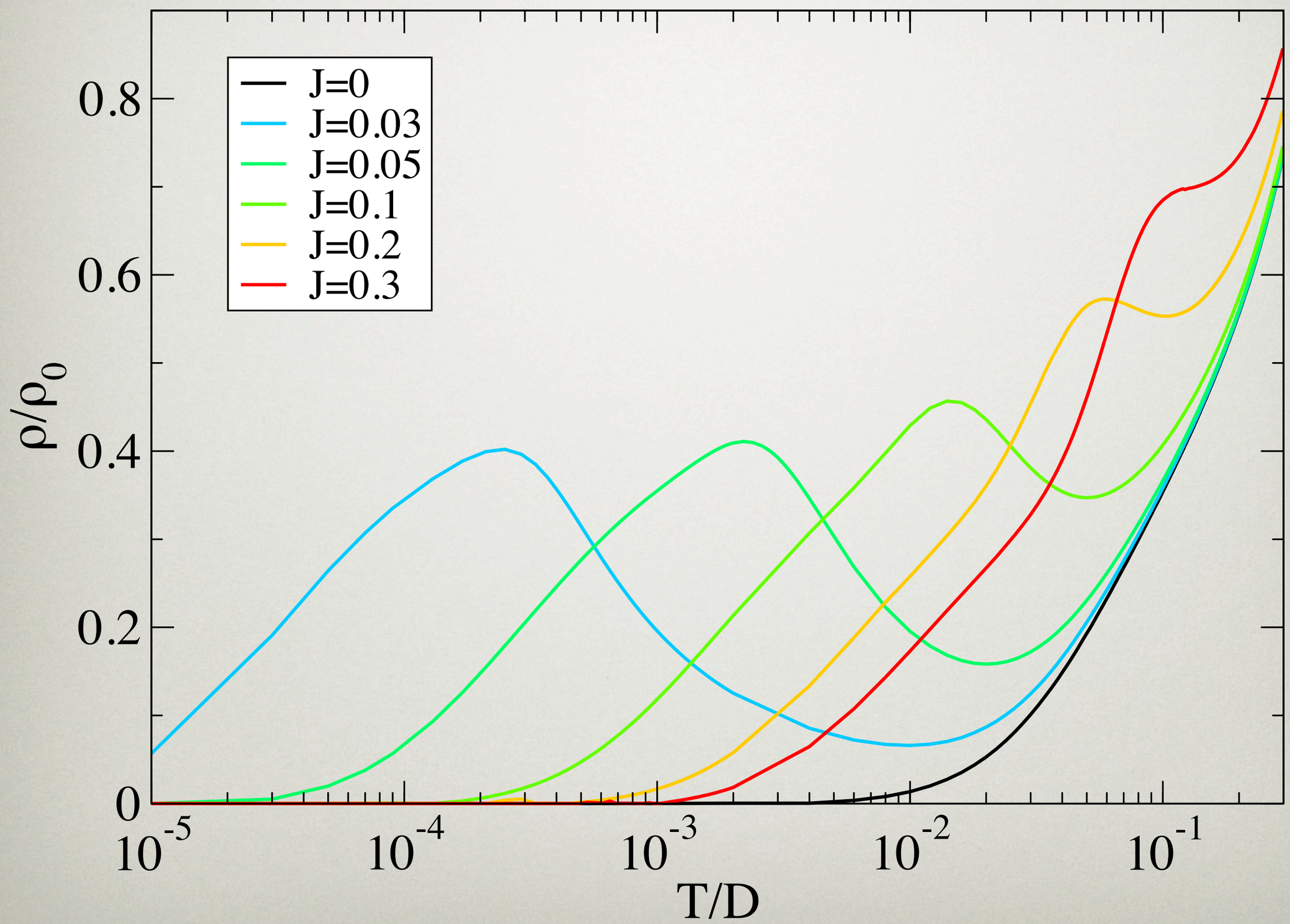




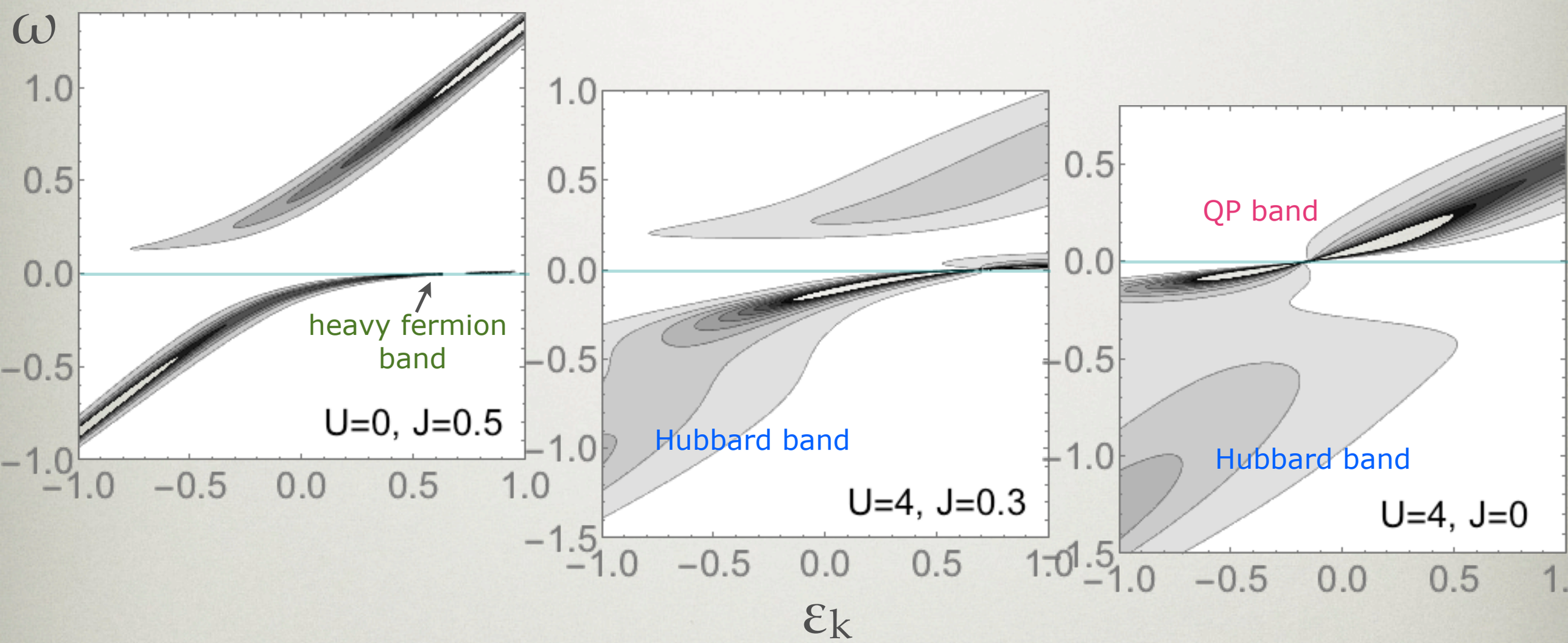
U=4, n=0.8


0.8
0.6
0.4
0.2
0
ρ/ρ0
0
0.05
0.1
0.15
0.2
0.25
0.3
T/D
J=0
J=0.03
J=0.05
J=0.1
J=0.2
J=0.3
increasing J

U=4, n=0.8



Momentum-resolved spectral functions



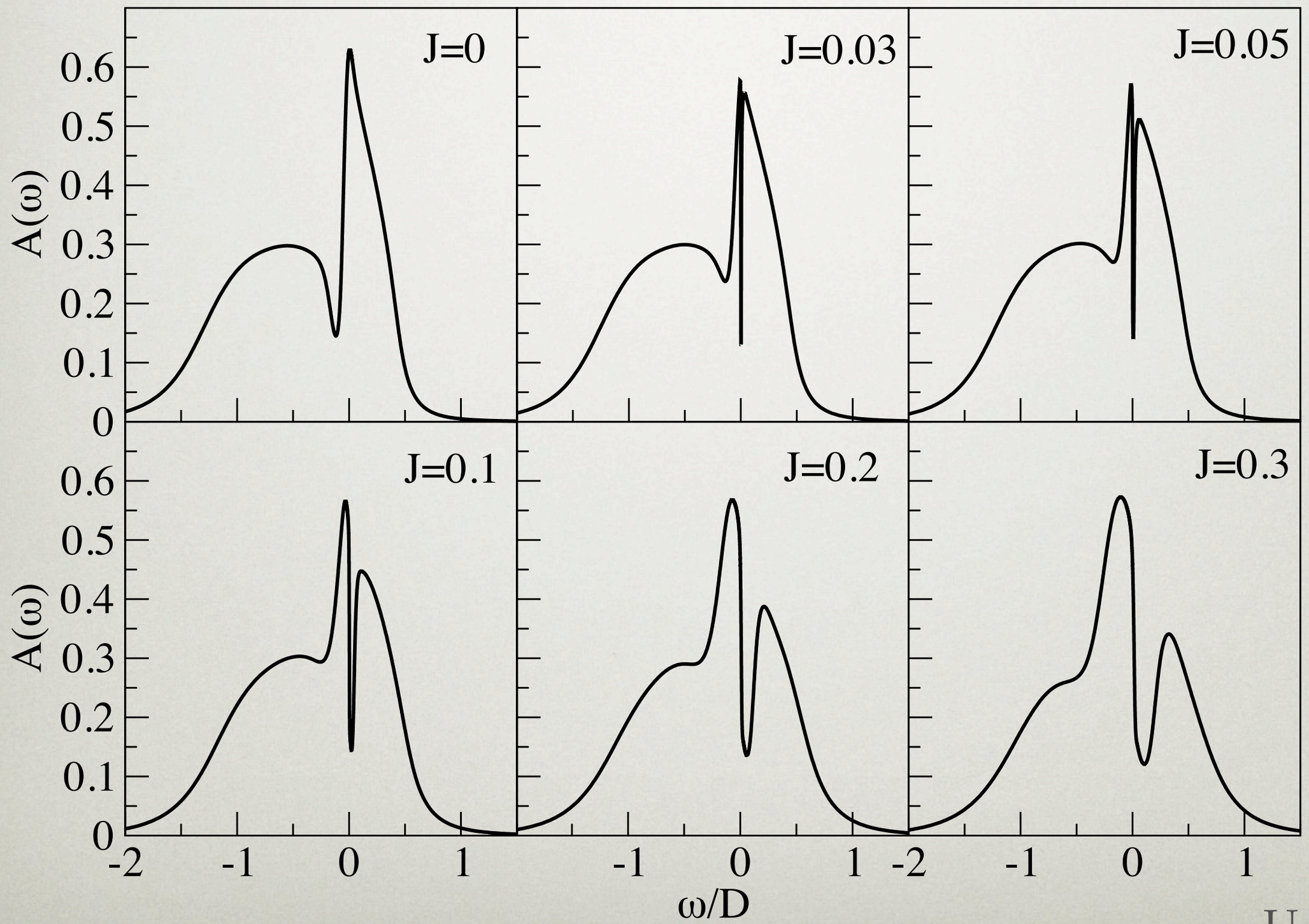
pure KLM

combined model

pure Hubbard model

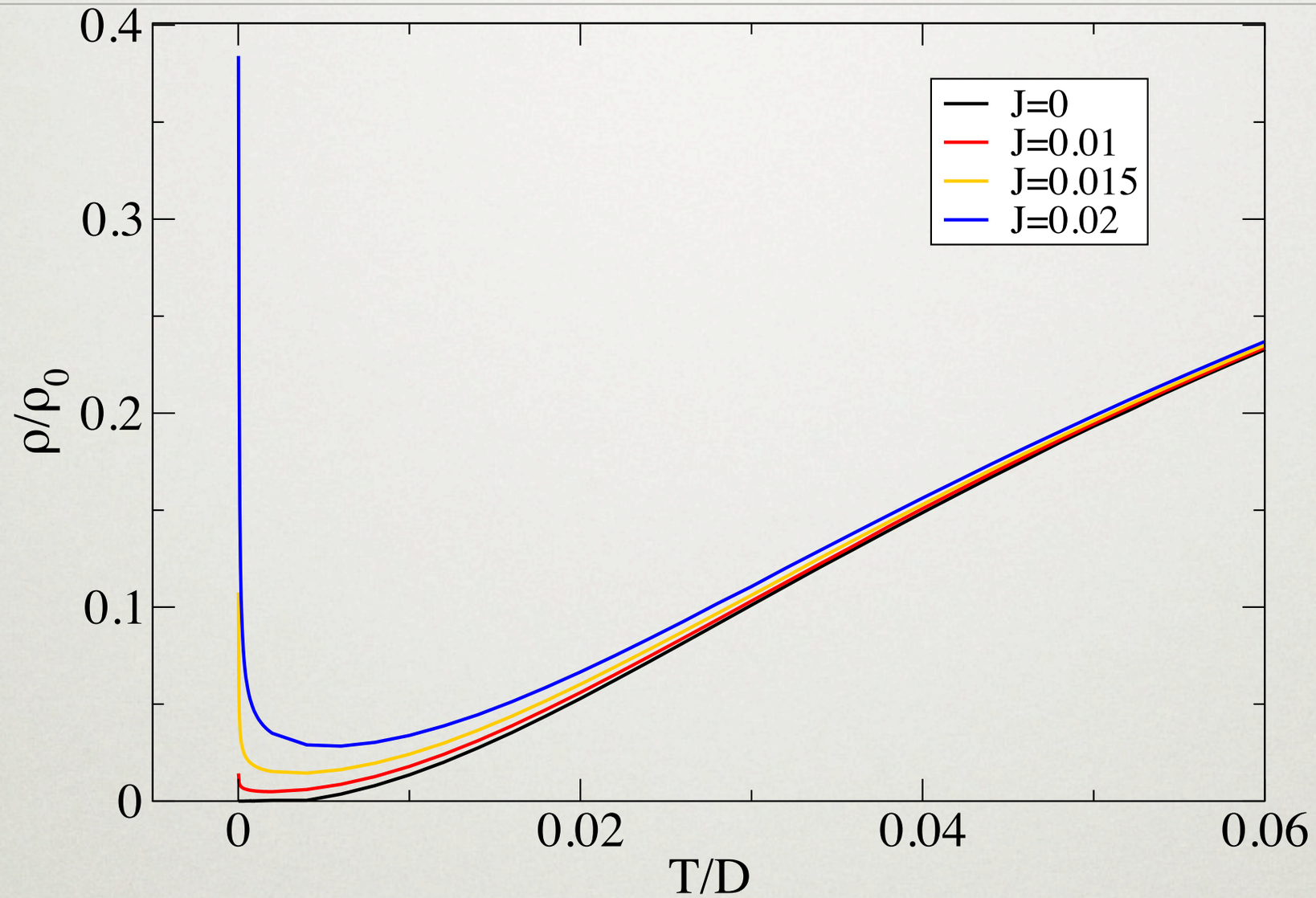
T=0

Spectral function: J-dependence



U=∞, n=0.8

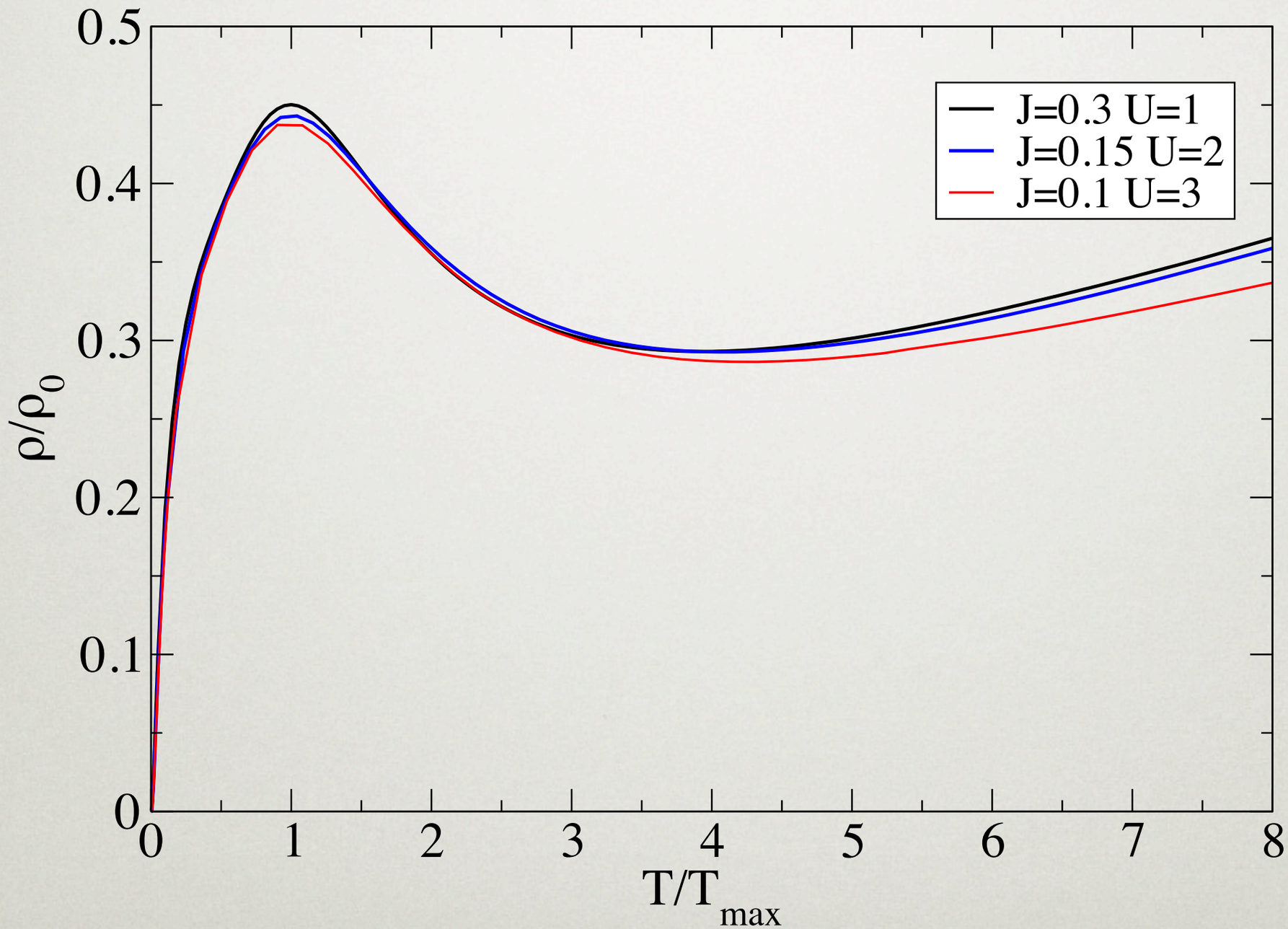
Limit of weakly coupled spins



Could this lead to seeming non-Fermi-liquid corrections in $CaCu_3Ru_4O_{12}$ at low temperatures?

A. Krimmel et al., Phys. Rev. B **78**, 165126 (2008)

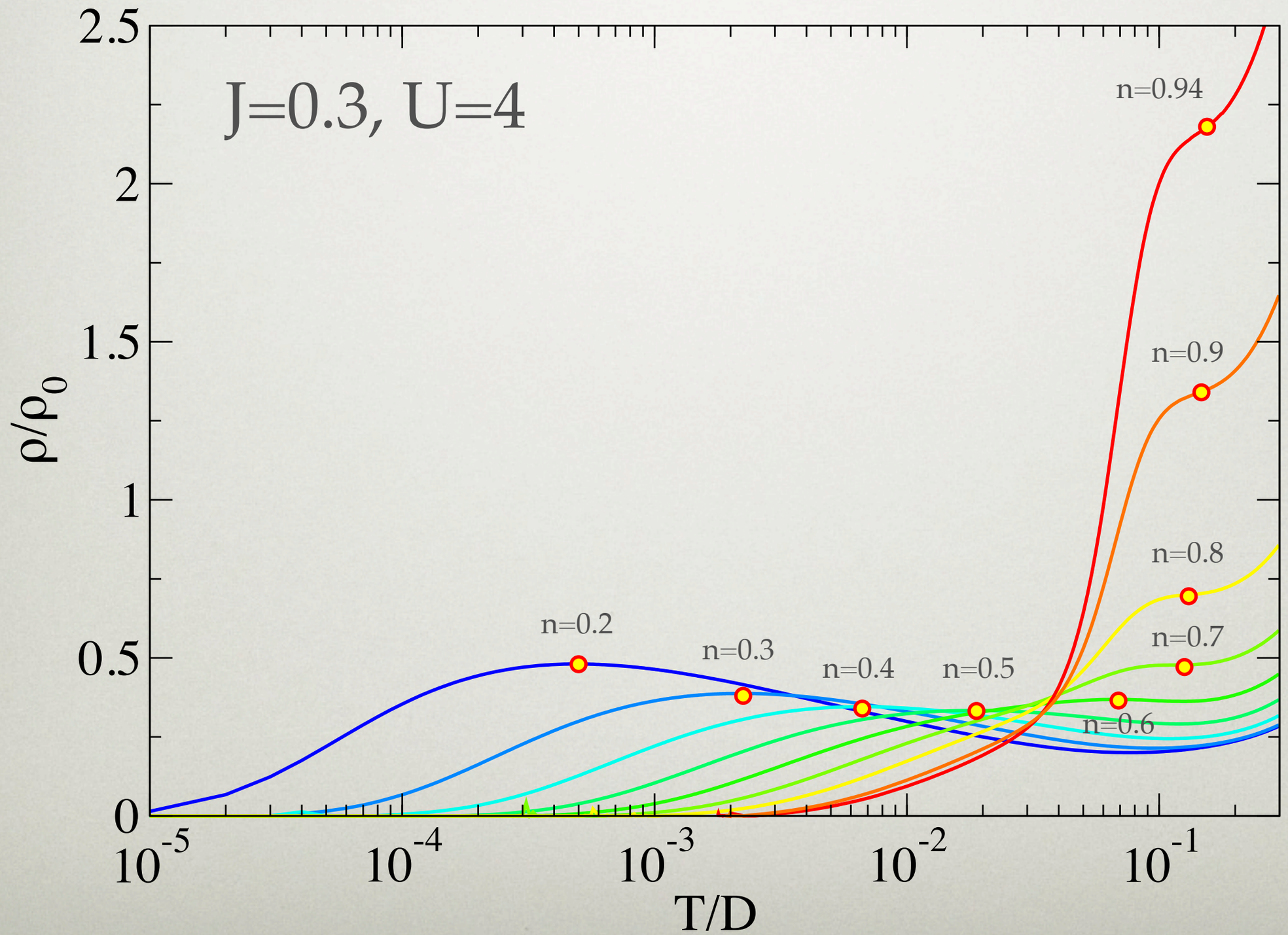
Universality for JU=const and n=const



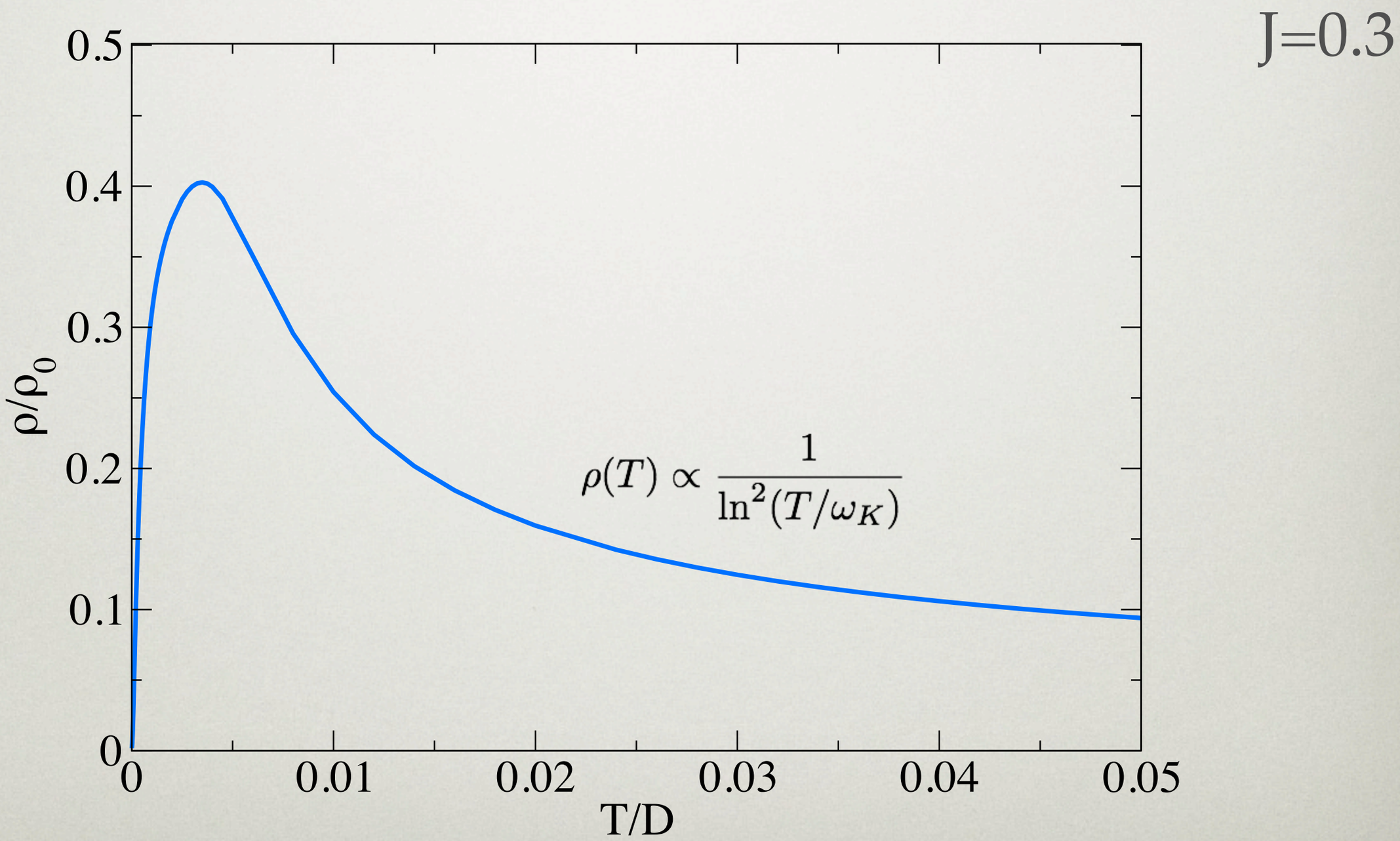
n=0.8

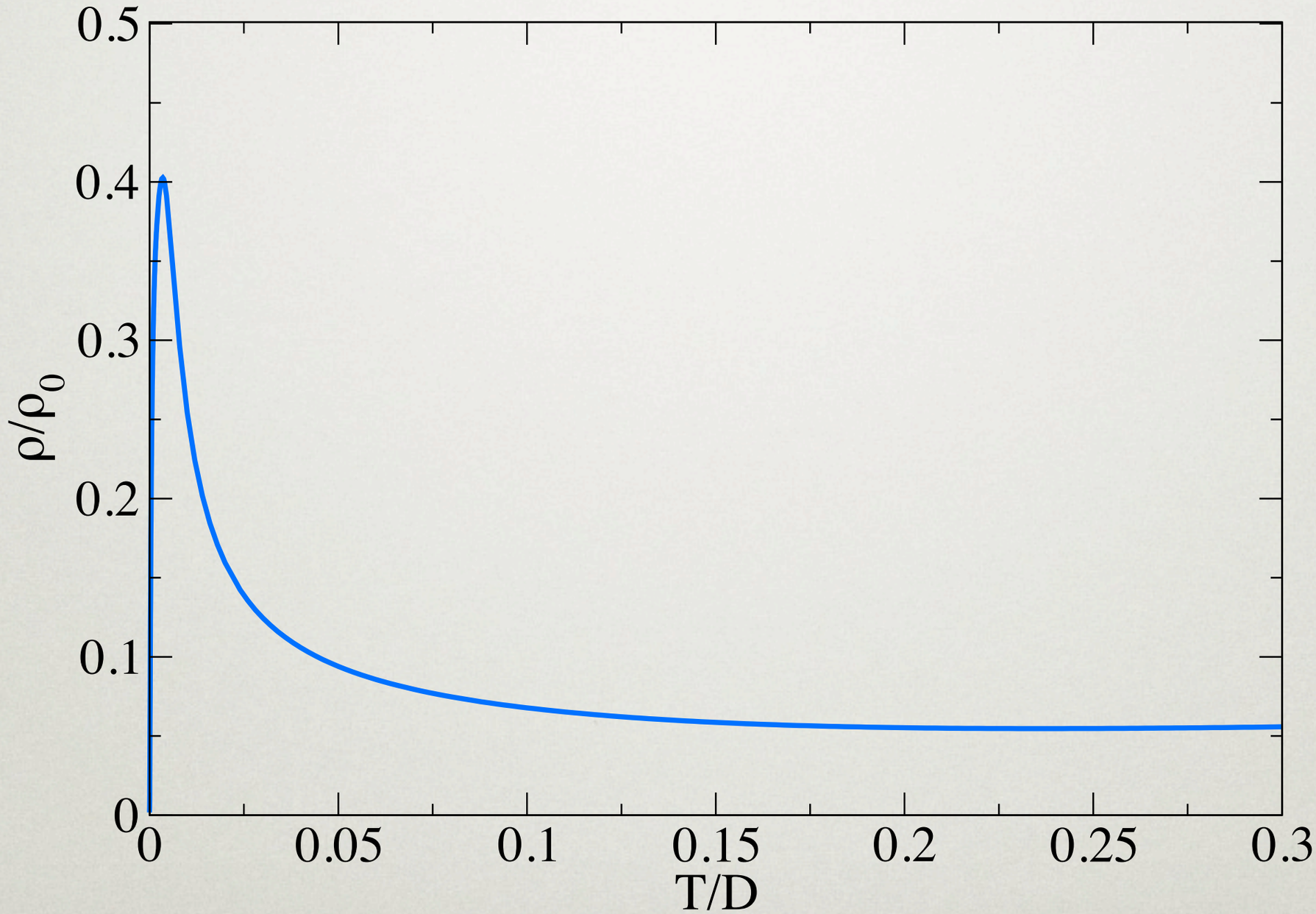
JU=const. □ $J/J_{s.e.}$=const. with $J_{s.e.}=4t^2/U$

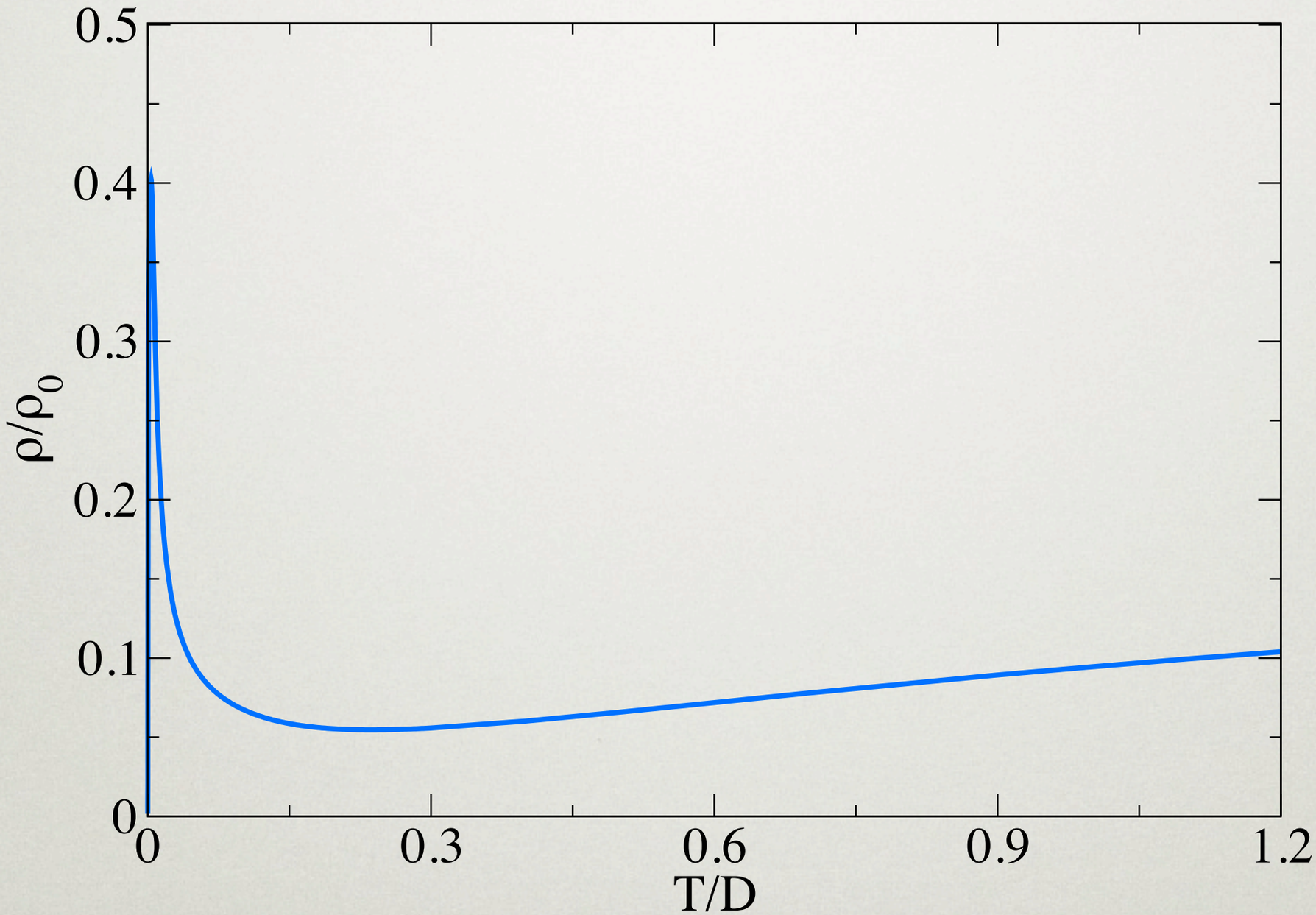
Doping dependence



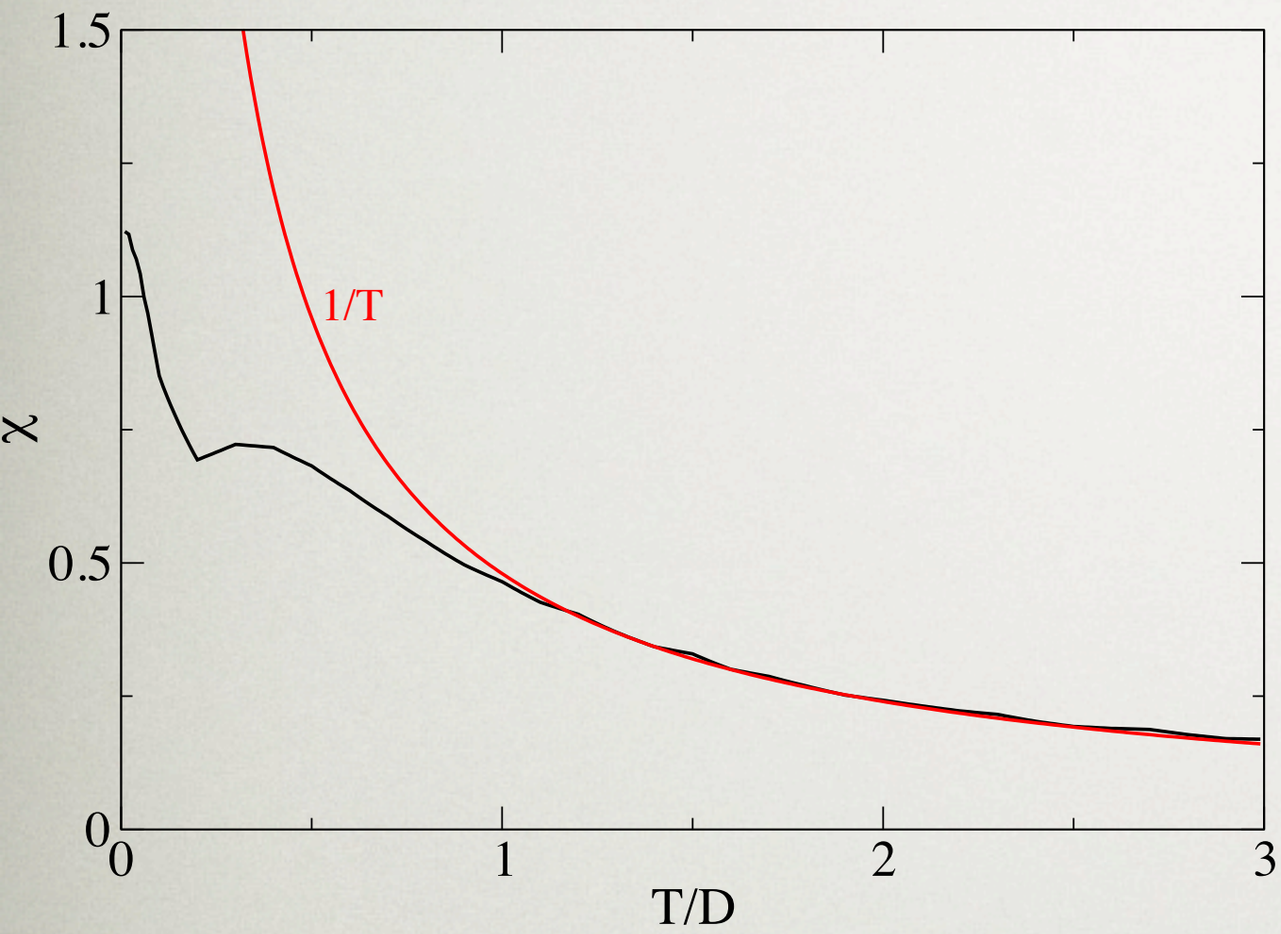
High-T asymptotics in pure KLM



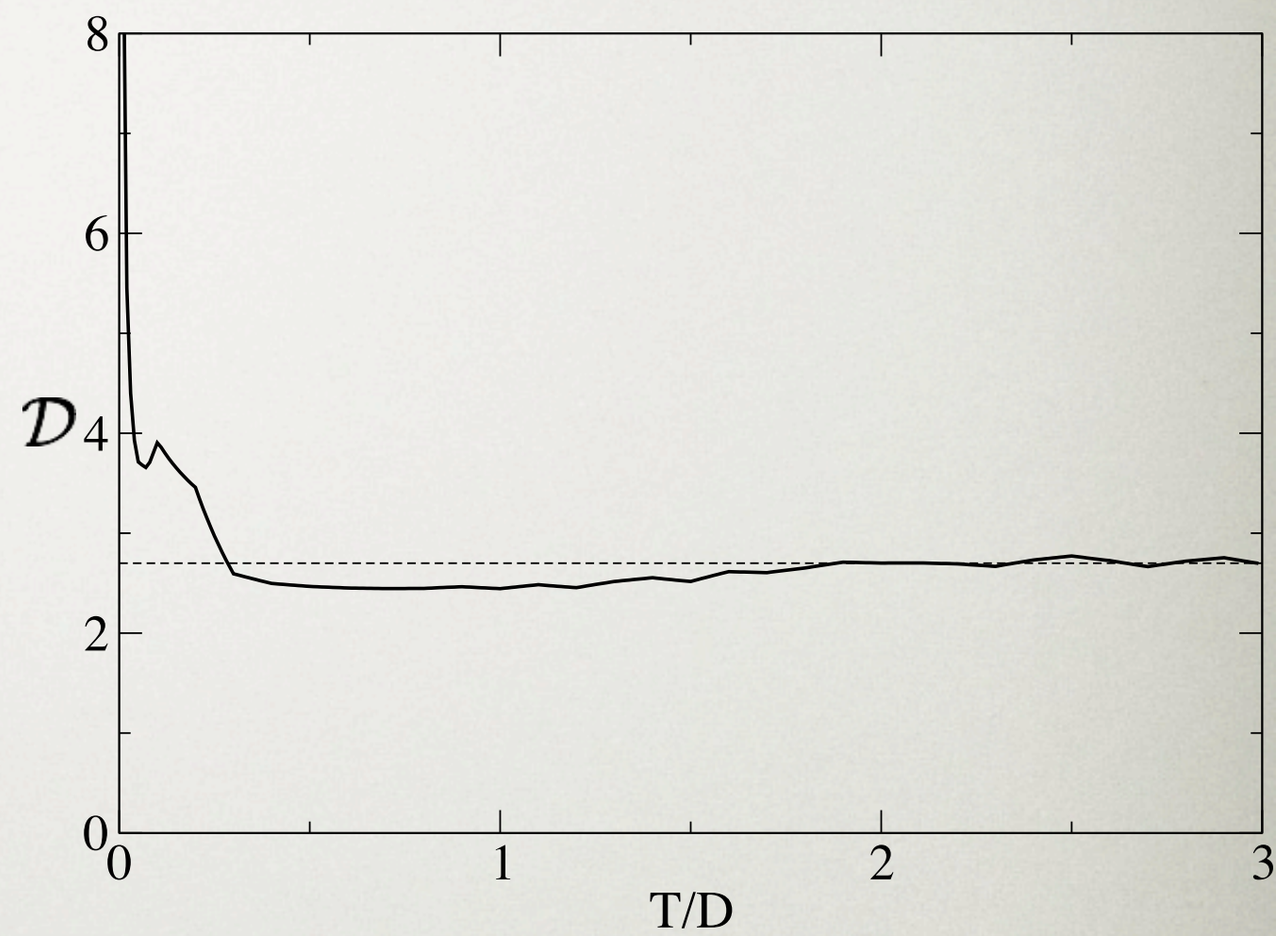

0.5
0.4
0.3
0.2
0.1
0
ρ/ρ0
0
0.05
0.1
0.15
0.2
0.25
0.3
T/D


0.5
0.4
0.3
0.2
0.1
0
ρ/ρ0
0
0.3
0.6
0.9
1.2
T/D

$$\sigma = \chi \mathcal{D}$$



charge susceptibility



diffusion constant

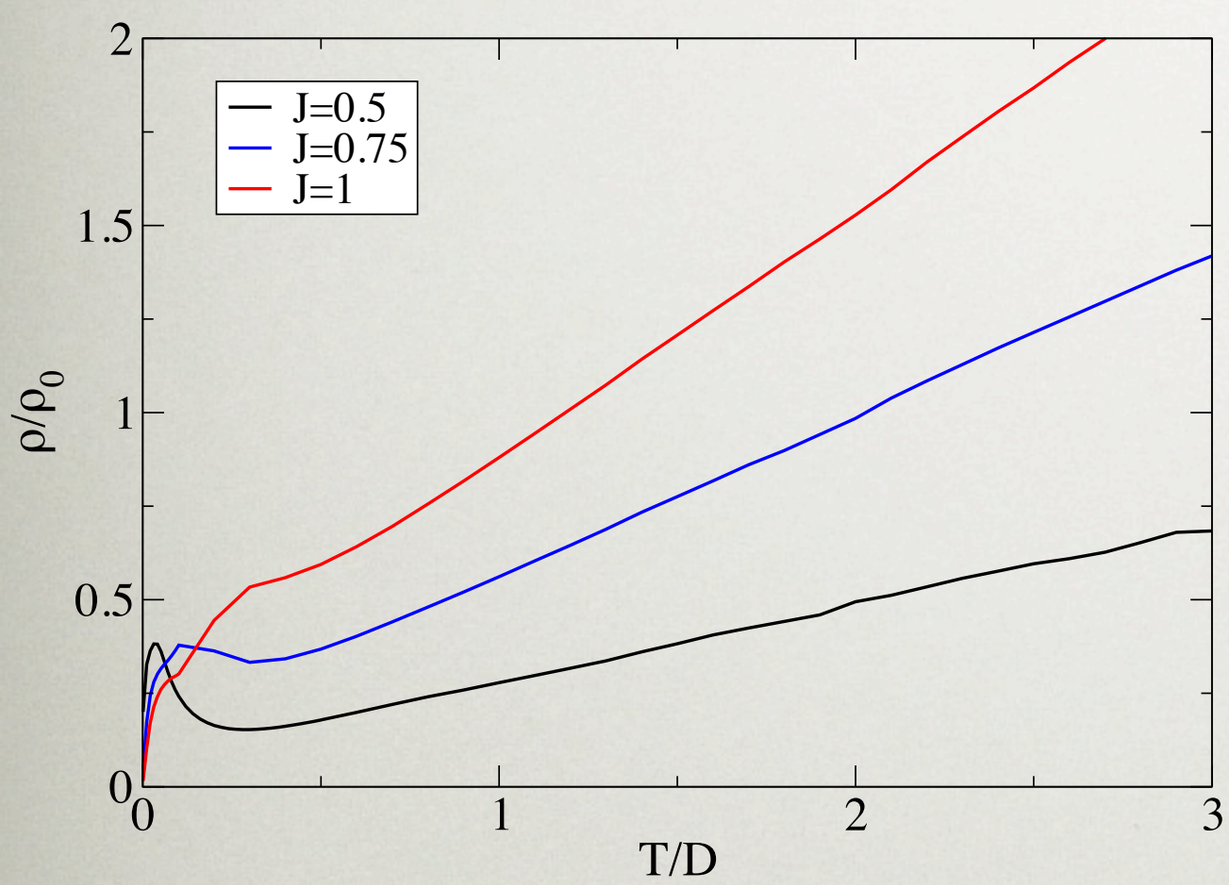
$$\chi(T) = \frac{\mathrm{d}n}{\mathrm{d}\mu} \propto \frac{1}{T}$$

$$\mathcal{D} \to \text{const.}$$

Calandra, Gunnarsson, EPL **61**, 88 (2003)
Perepelitsky et al., PRB **94**, 235115 (2016)
Kokalj, PRB **95**, 041110 (2017)

High-T asymptotics

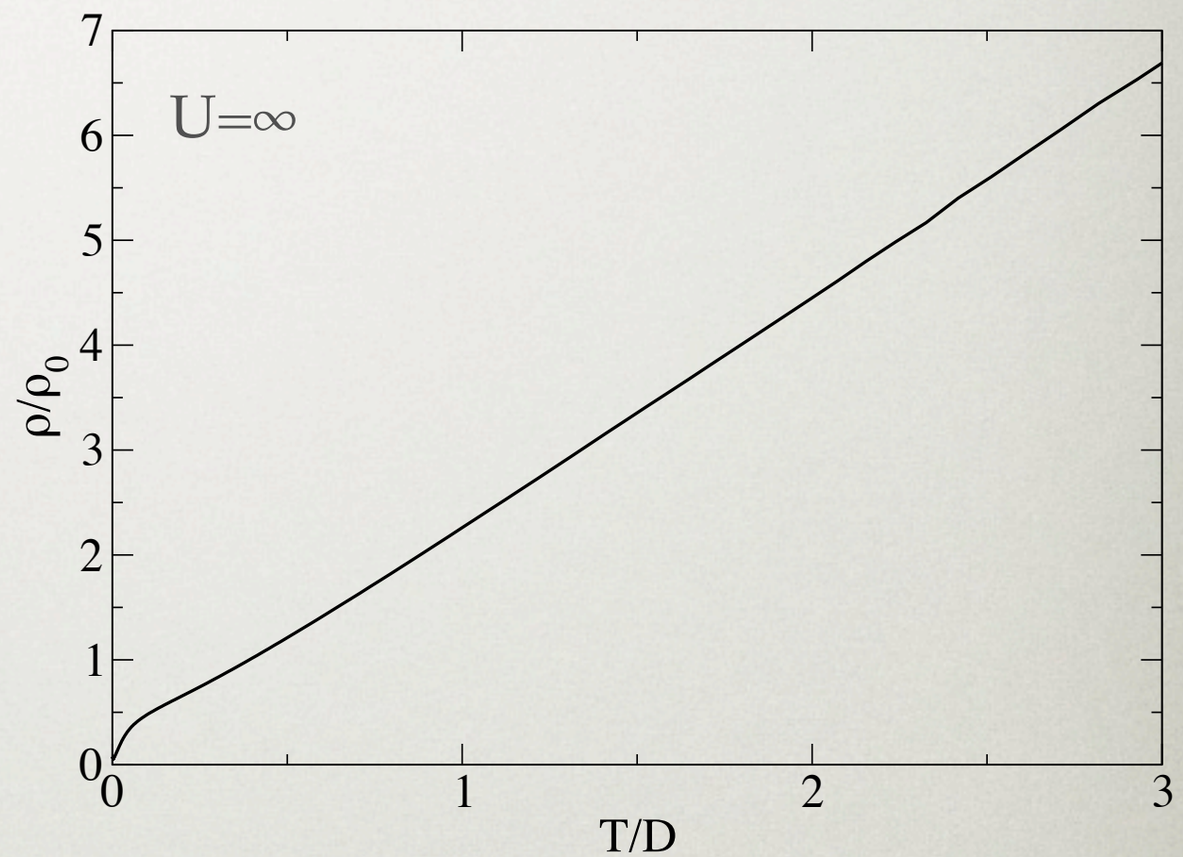
U=0 (pure KLM)



ϱ linear in T with J-dependent slope

$$\rho_J \propto \frac{J^2}{T}$$

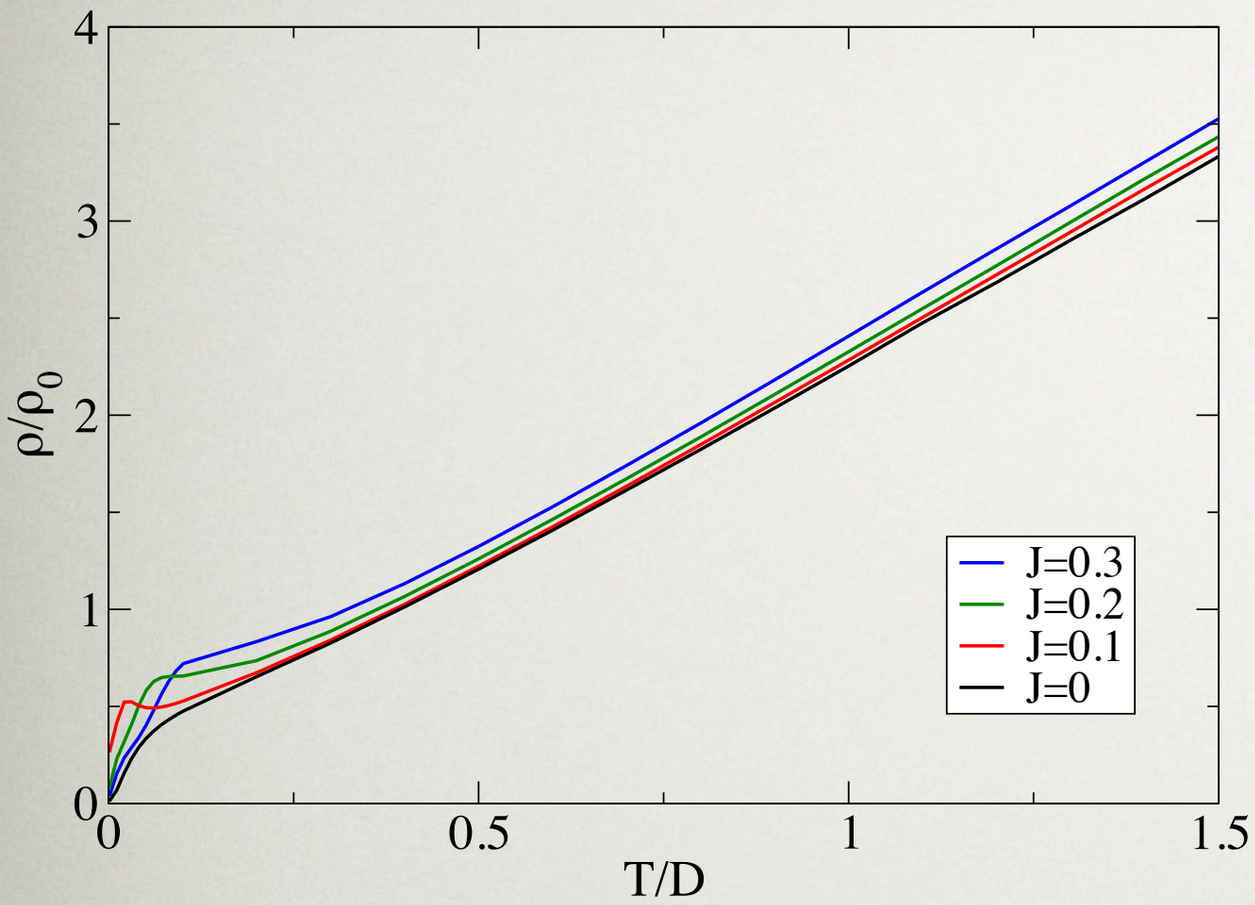
J=0 (pure Hubbard)



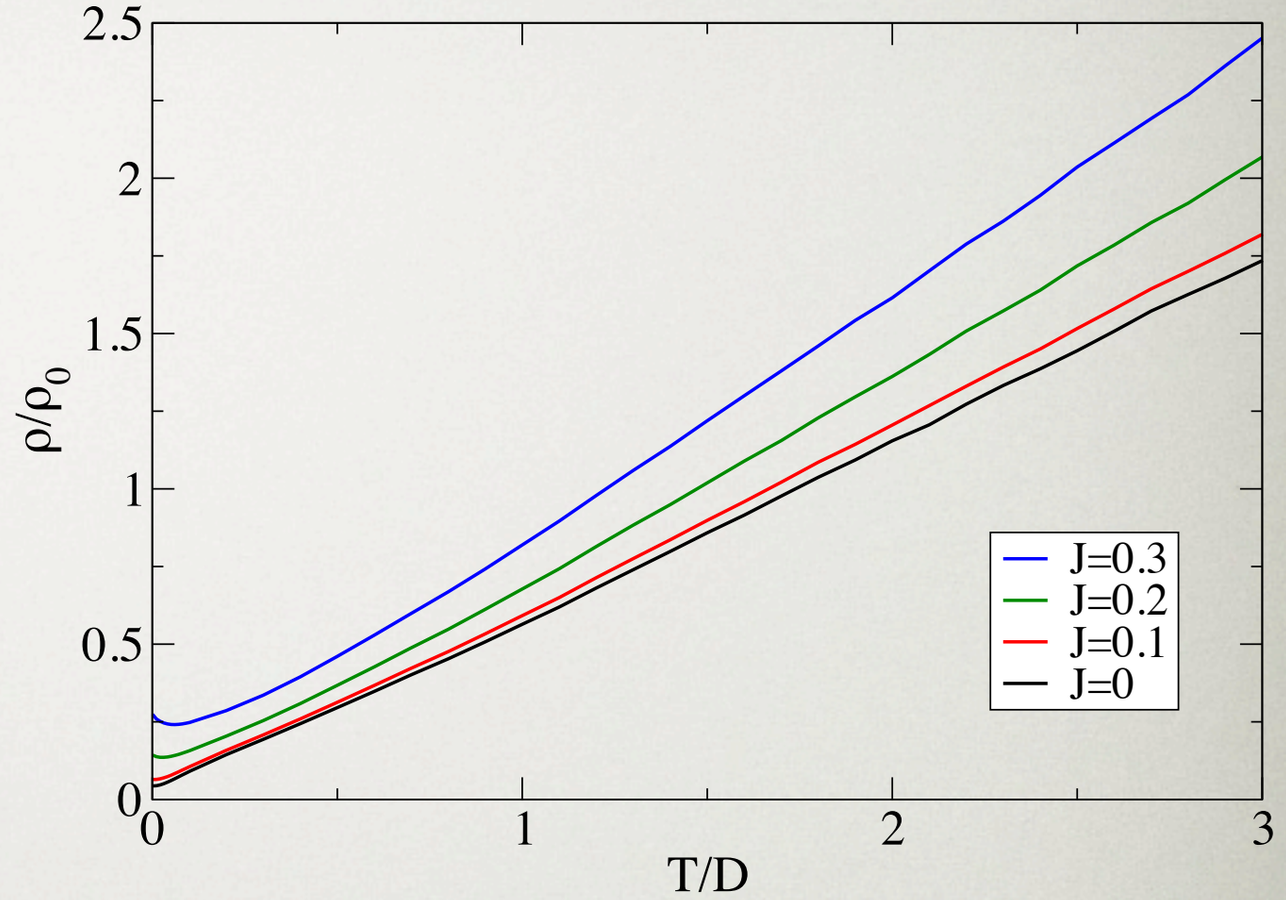
ϱ linear in T with n-dependent slope

$$\rho_U \propto \frac{1}{1-n} \times \frac{1}{T}$$

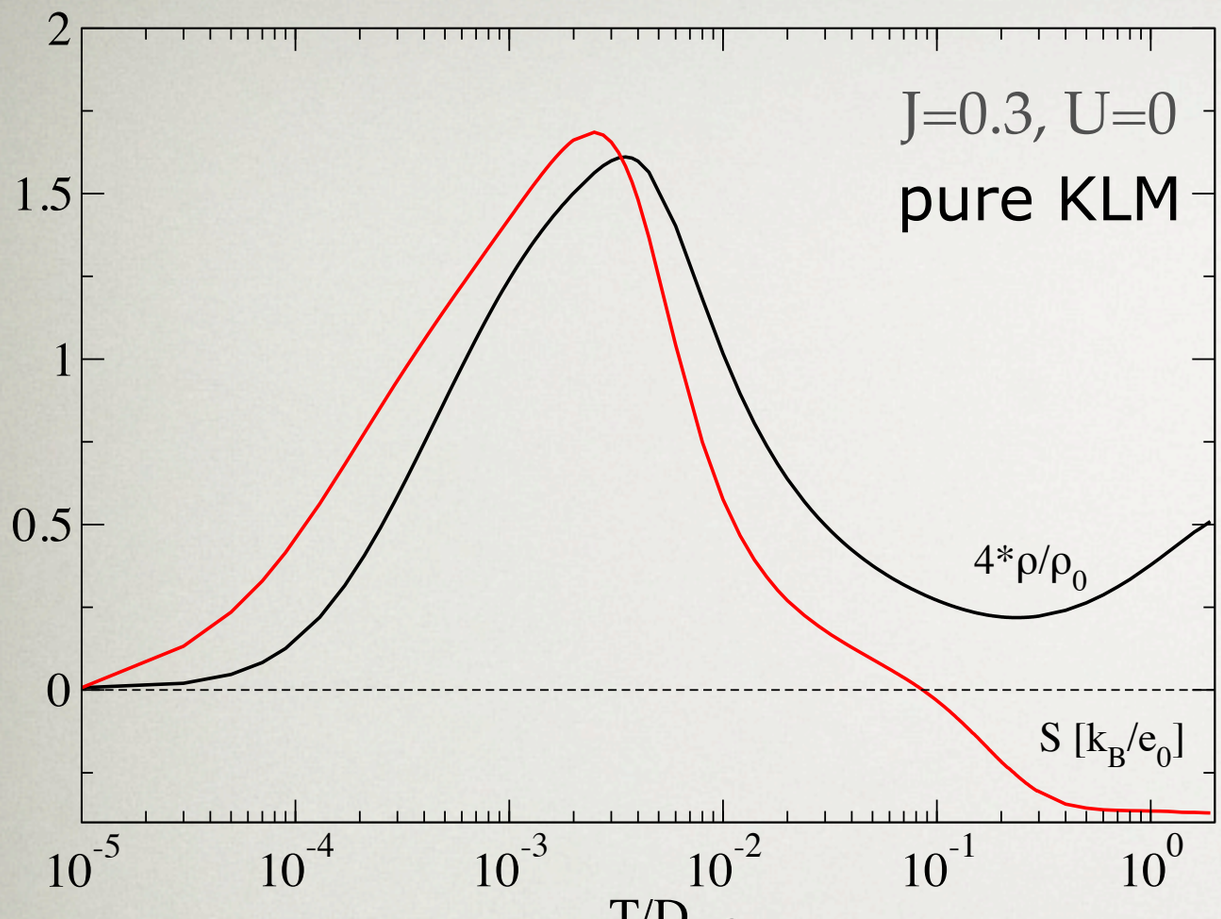
U=∞, n=0.8

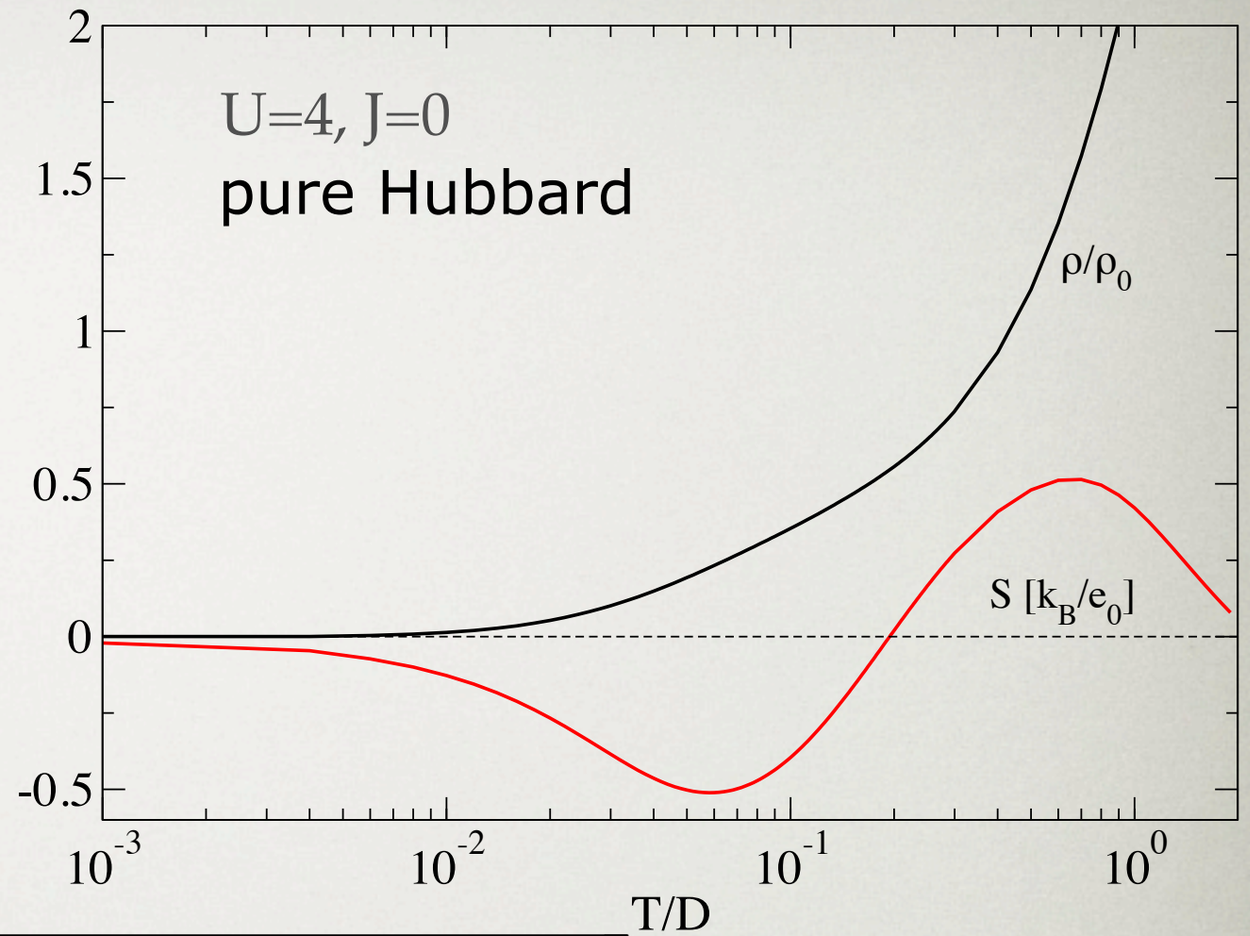


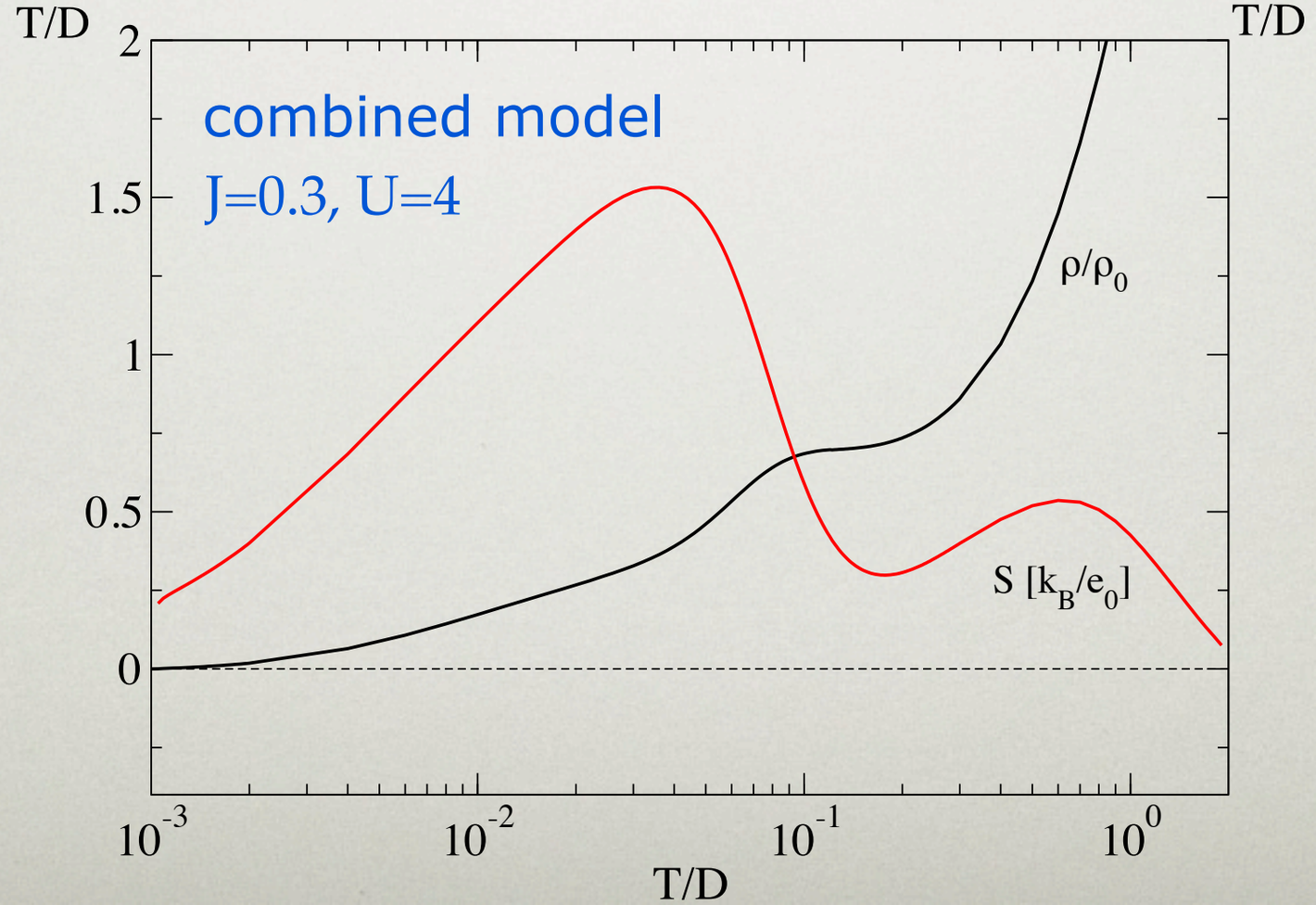
U=∞, n=0.2



additive linear-in-T contributions


J=0.3, U=0
pure KLM
4*ρ/ρ0
S [kB/e0]
T/D

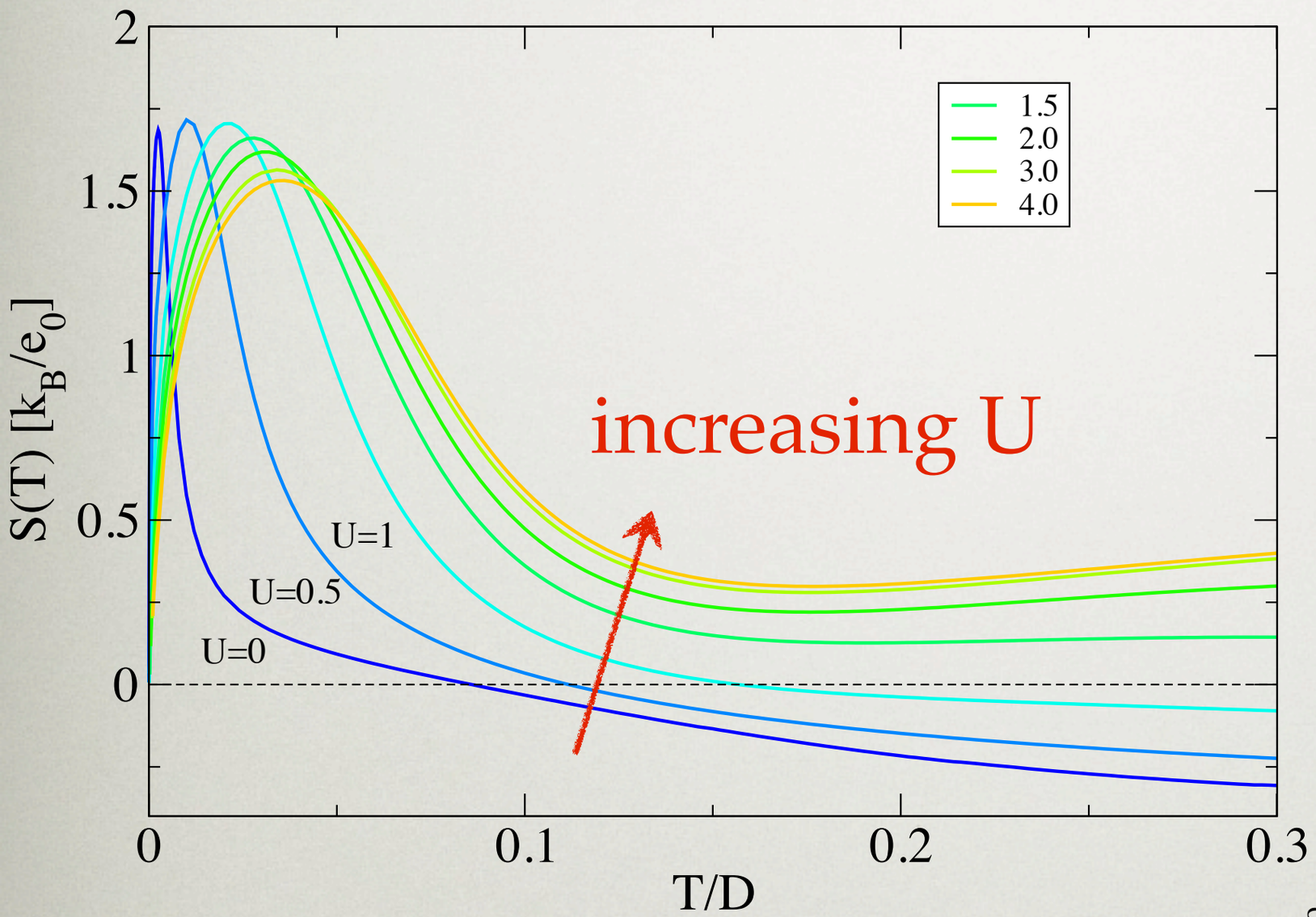

U=4, J=0
pure Hubbard
ρ/ρ0
S [kB/e0]
T/D

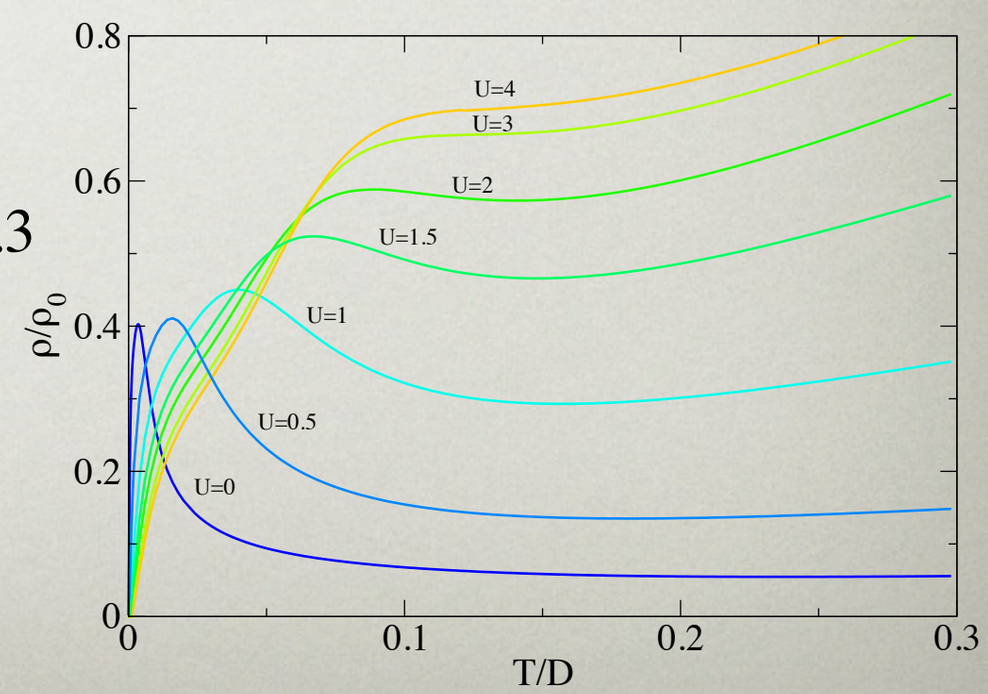

combined model
J=0.3, U=4
ρ/ρ0
S [kB/e0]
T/D

n=0.8

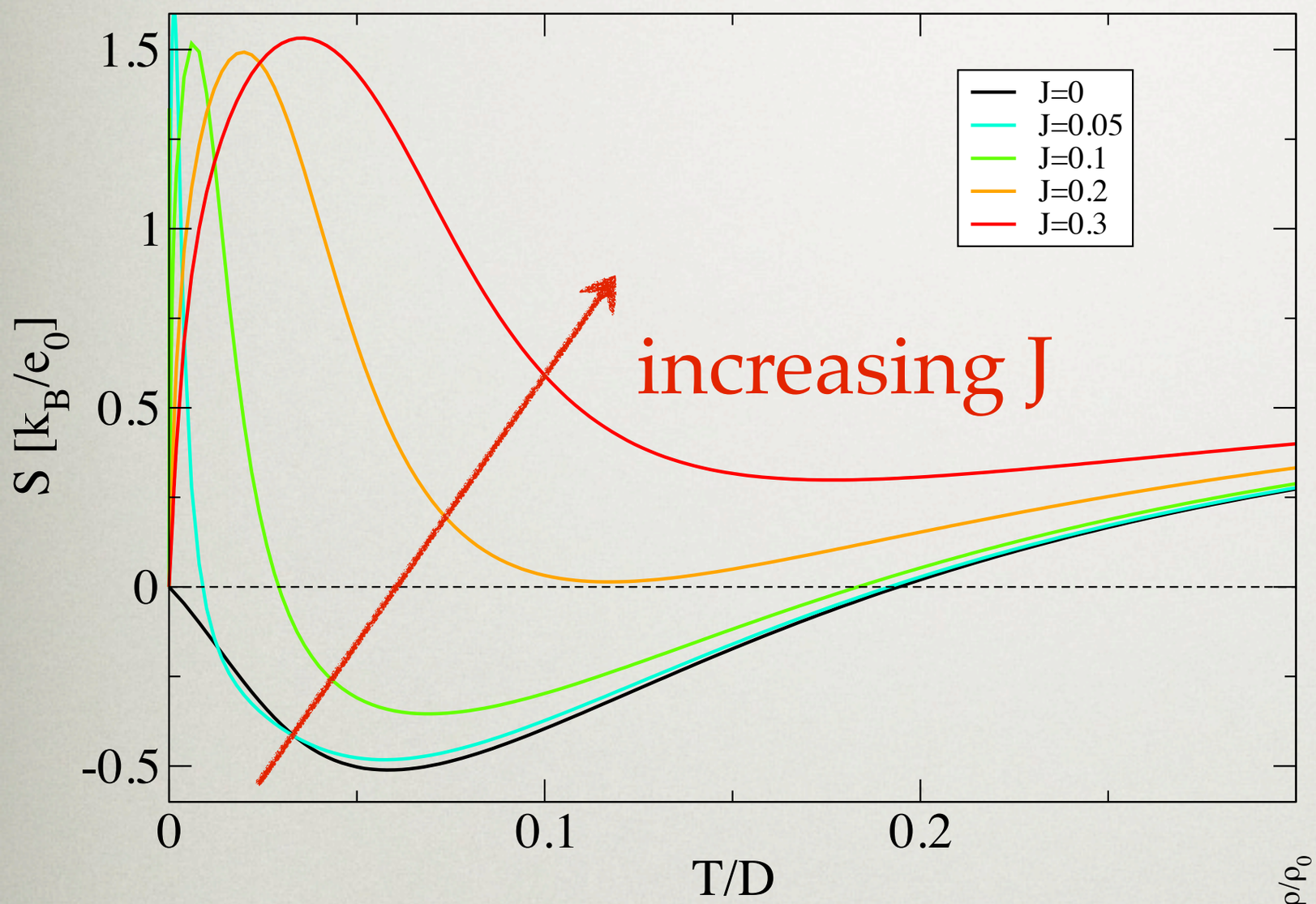
Effect of U on thermopower

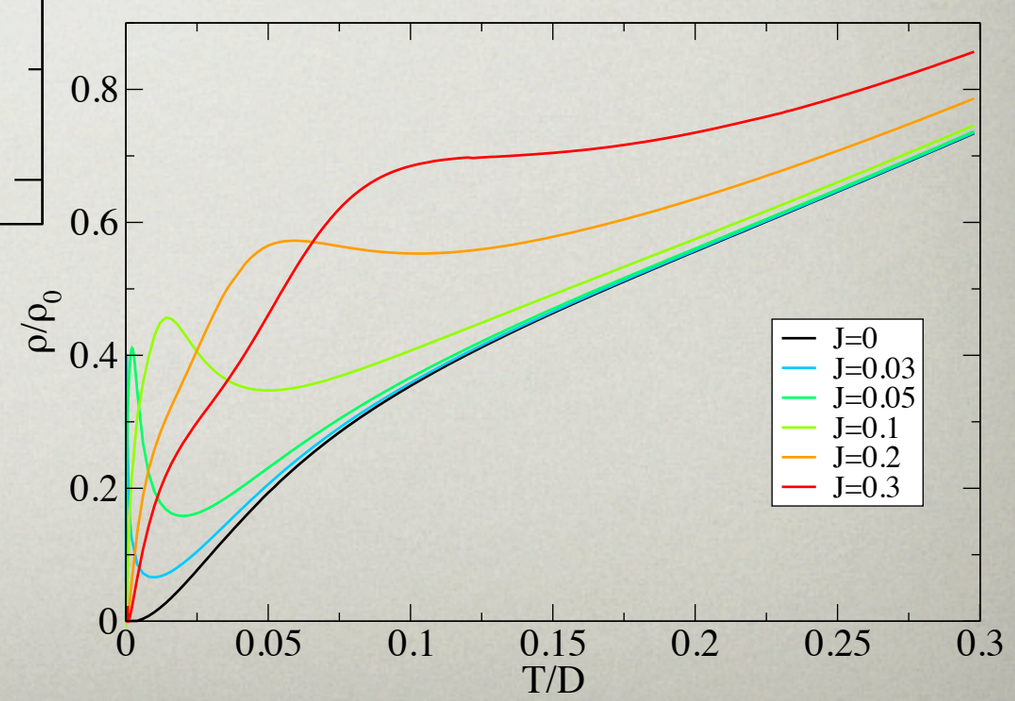
J=0.3, n=0.8





Effect of J on thermopower





Summary

- a family of models interpolating between pure HM and pure KLM
- a resistivity peak at T_{max} that evolves into a kink for large J & U
- universality for n=const. and UJ=const.
- thermopower with two positive peaks for large J & U