The Structure of the Hubbard Model Pairing Interaction

KITP June 2009

Thomas Maier ORNL
Mark Jarrell LSU
Doug Scalapino UCSB

Center for Nanophase Material Science
Oak Ridge National Laboratory, DOE

The question of what is the pairing mechanism responsible for high Tc superconductivity will be decided experimentally.

The question of what is the pairing mechanism responsible for high Tc superconductivity will be decided experimentally.

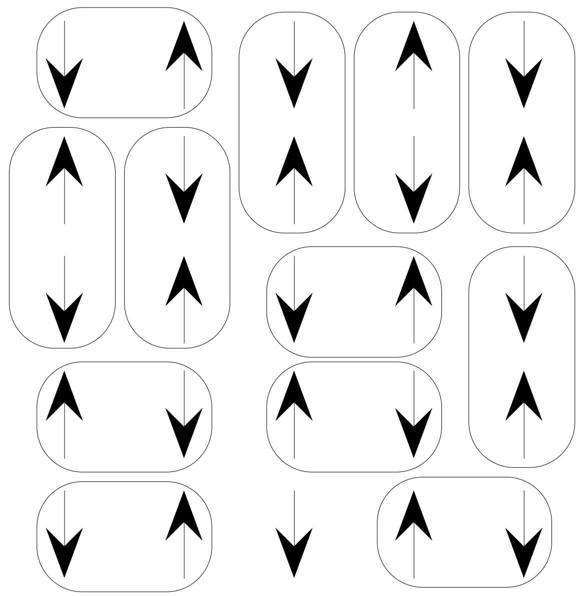
However, we should be able to understand the pairing interaction for models such as the Hubbard and t-J models which exhibit properties similar to the cuprates.

The question of what is the pairing mechanism responsible for high Tc superconductivity will be decided experimentally.

However, we should be able to understand the pairing interaction for models such as the Hubbard and t-J models which exhibit properties similar to the cuprates.

But even among those who believe that these models contain much of the essential physics of the cuprates, there are different views regarding the nature of the pairing interaction.

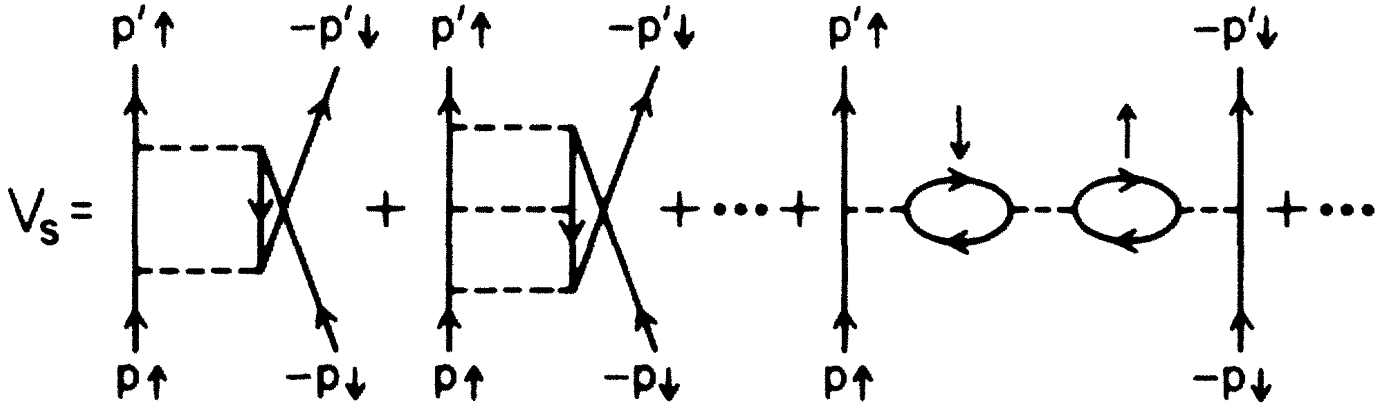
RVB postulates a liquid of spin singlets from which superconductivity arises.



"The Resonating Valence Bond State in La2CuO4 and Superconductivity"

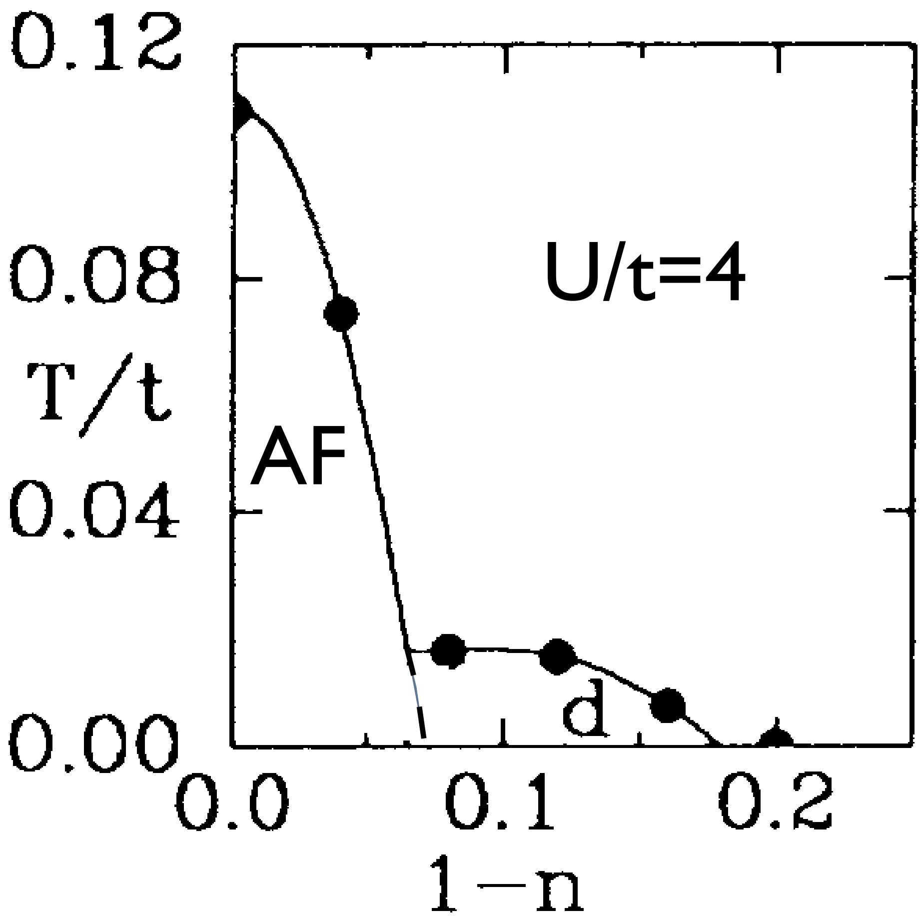
P.W. Anderson, Science 235,1196 (1987)

Spin-fluctuation exchange mechanism



K. Miyake, S. Schmitt-Rink and C. Varma, PRB 34, 6554 (1986)

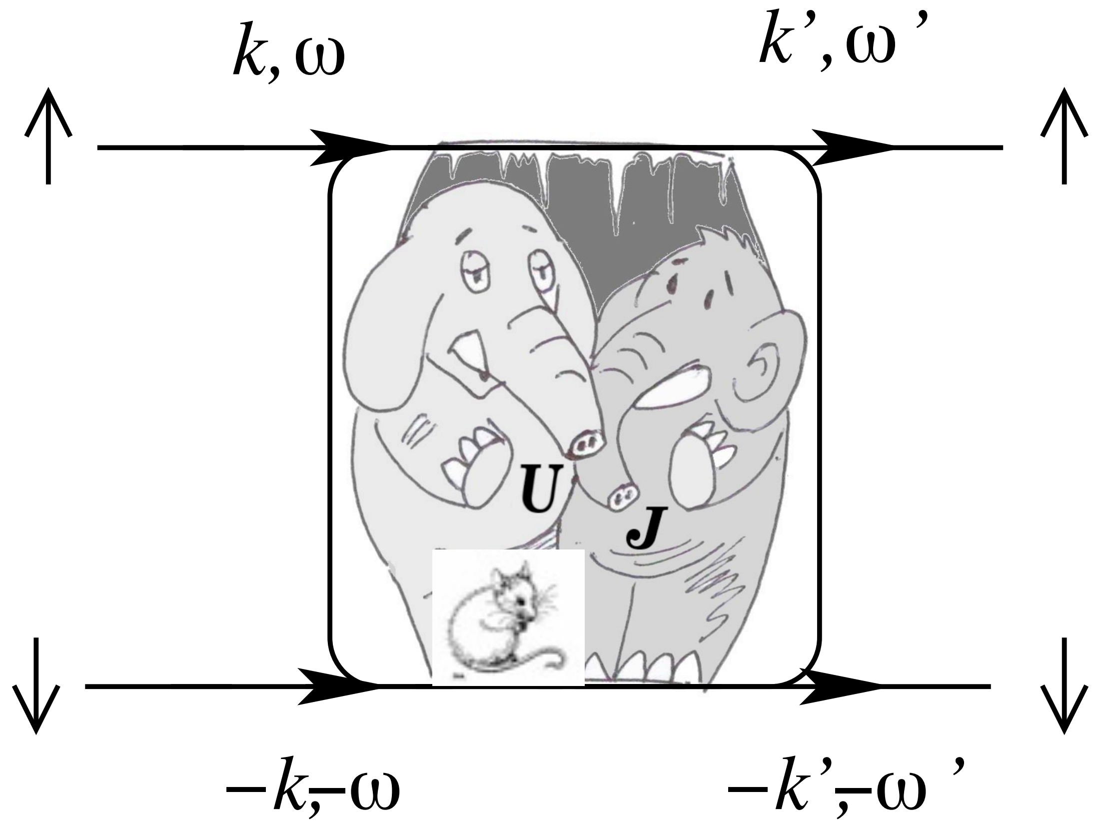
D. Scalapino, E. Loh, Jr., J. Hirsch, PRB 34, 8190 (1986)



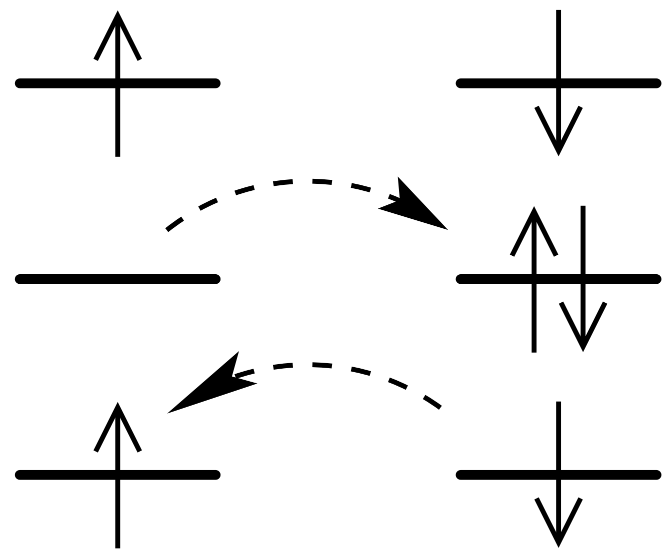
Bickers, Scalapino and White PRL (1989)

“we have a mammoth and an elephant in our refrigerator---do we care much if there is also a mouse?”

P.W. Anderson Science 2007



$$J = \frac{4t^2}{U}$$



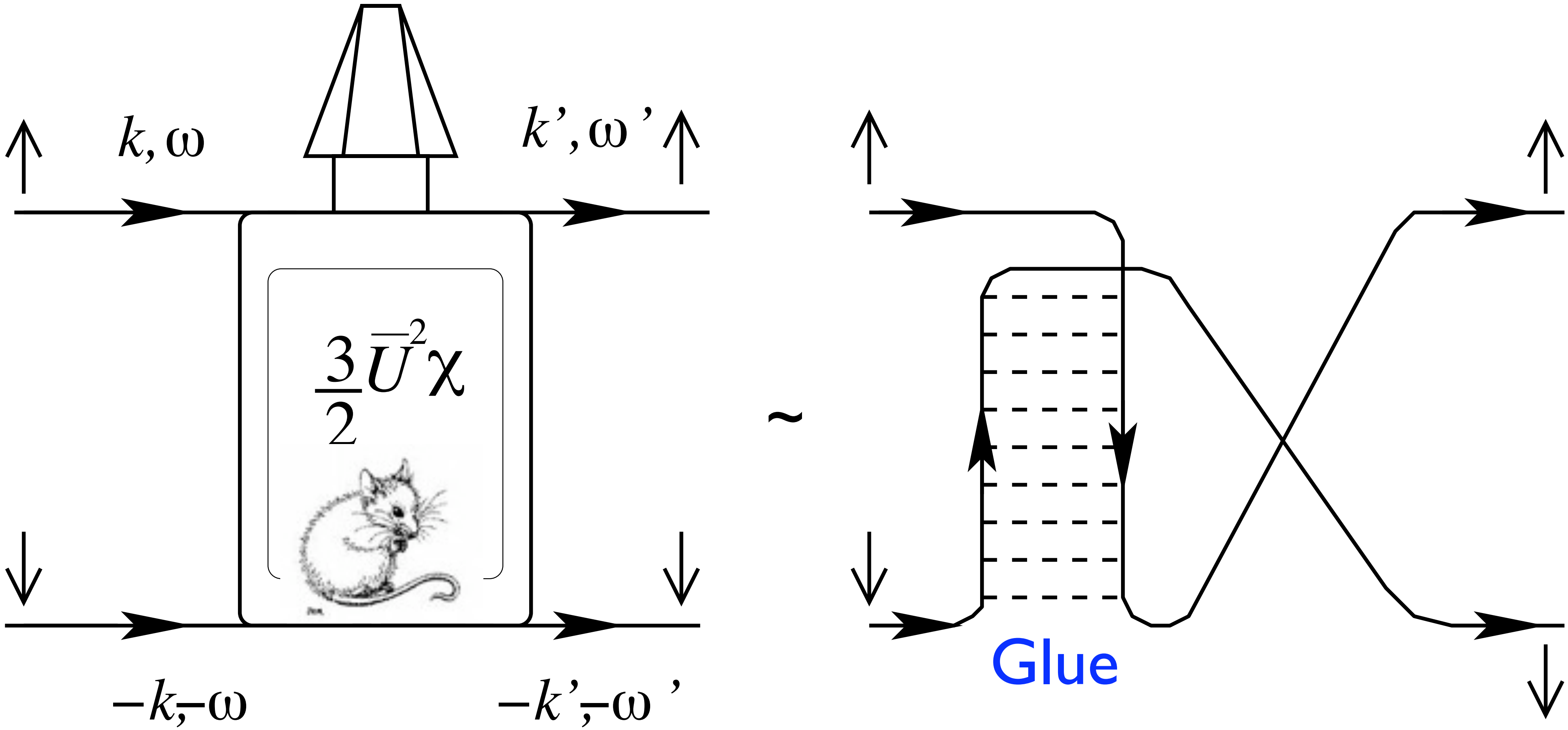
$$V_{\mathrm{RVB}} = J\,(\cos k_x - \cos k_y)(\cos k'_x - \cos k'_y)$$

If $\Gamma^{pp}_{\text{RVB}} \approx J(cosk_x - cosk_y)(cosk'_x - cosk'_y)$

with the dynamics of J set by the Mott scale U

$$J = 4t^2/U$$

the interaction is non-retarded and one would not speak of a "glue".



$$V_{SF} = \frac{3}{2}\bar{U}^2 \chi(k-k', \omega-\omega')$$

If Γ^{pp} has a frequency dependence like the spin susceptibility, it is retarded and one could say that spin-fluctuations provide the pairing "glue".

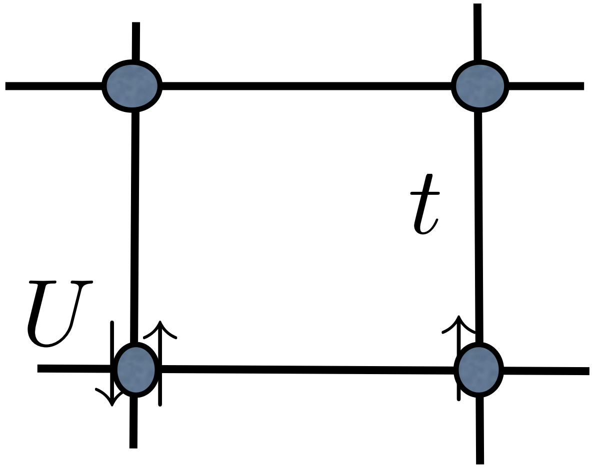
$$\Gamma^{pp}(k,\omega;k',\omega') \approx \frac{3}{2}\bar{U}^2\chi(k-k',\omega-\omega')$$

Numerical results

DCA T. Maier et al , Rev Mod Phys 77, 10271 (2005)

C-DMFT G. Kotliar et al, Rev Mod Phys 78, 865 (2006)

The Hubbard Model

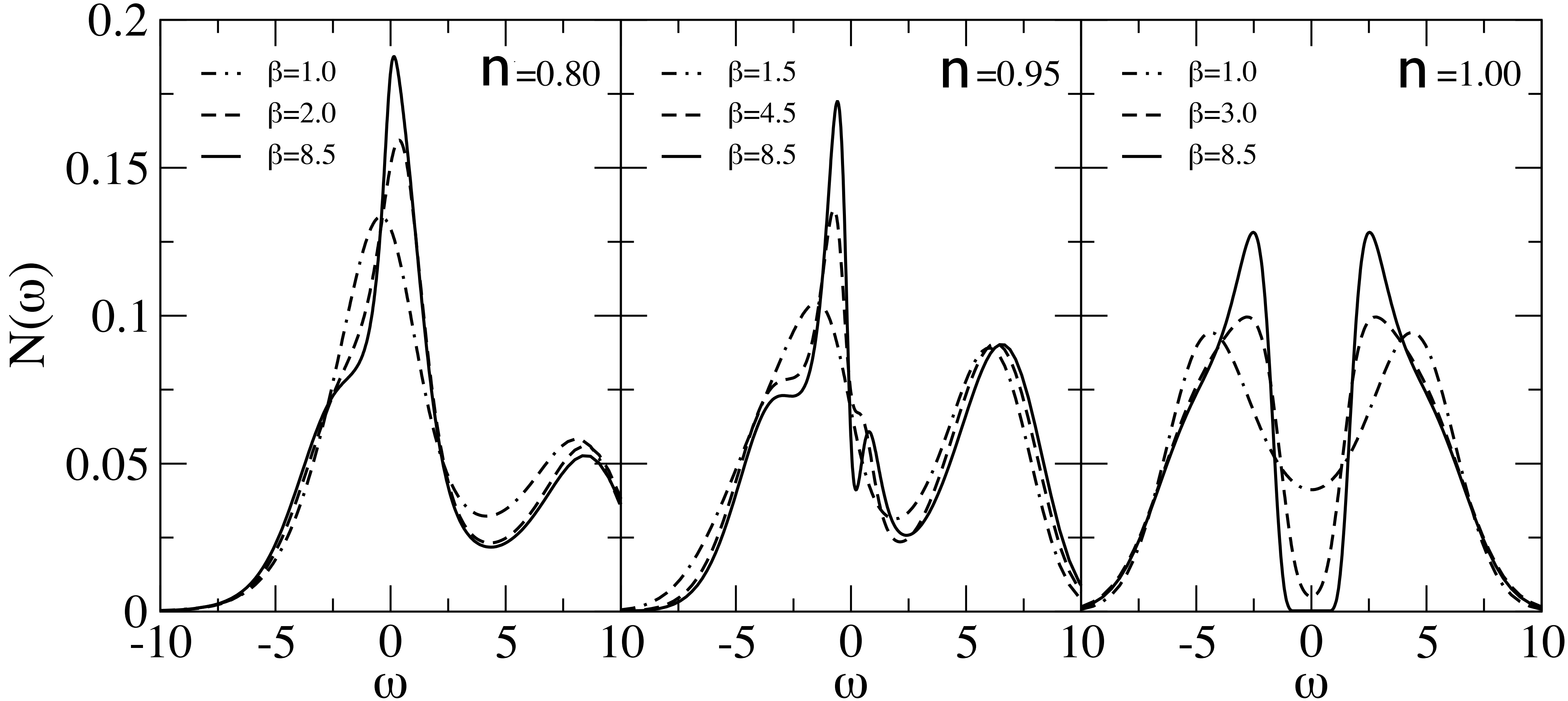


$$H = -t \sum_{<i,j>\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

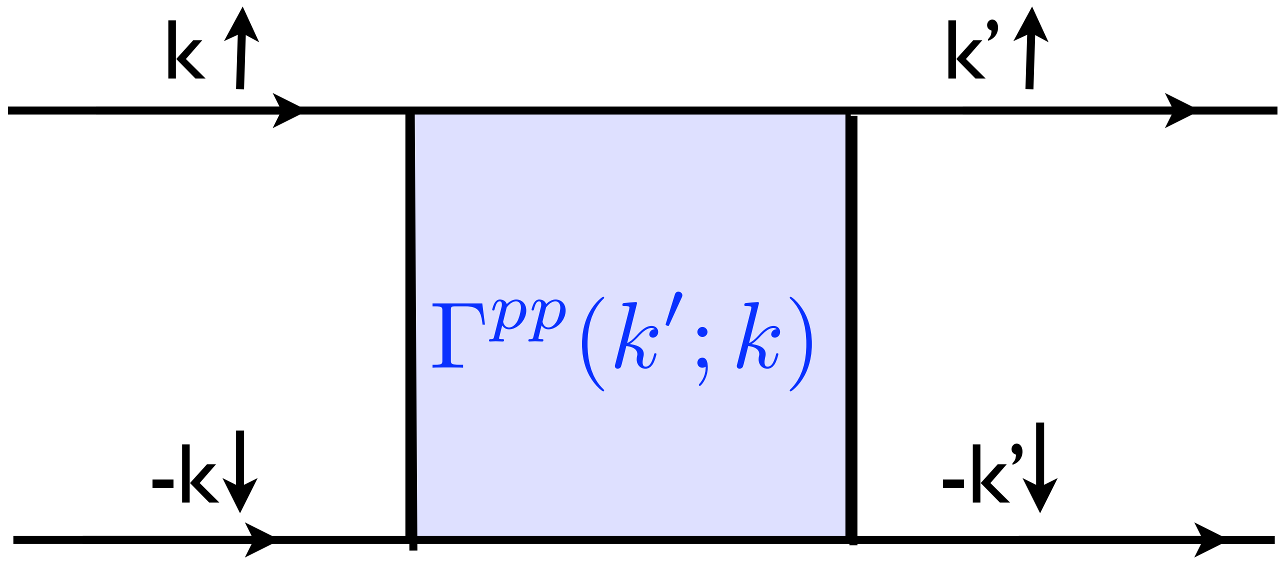
U/t $\quad$ n =1-x

$$U = 8t$$

$$J = 4t^2/U = 0.5t$$



The effective pairing interaction is given by the irreducible particle-particle vertex

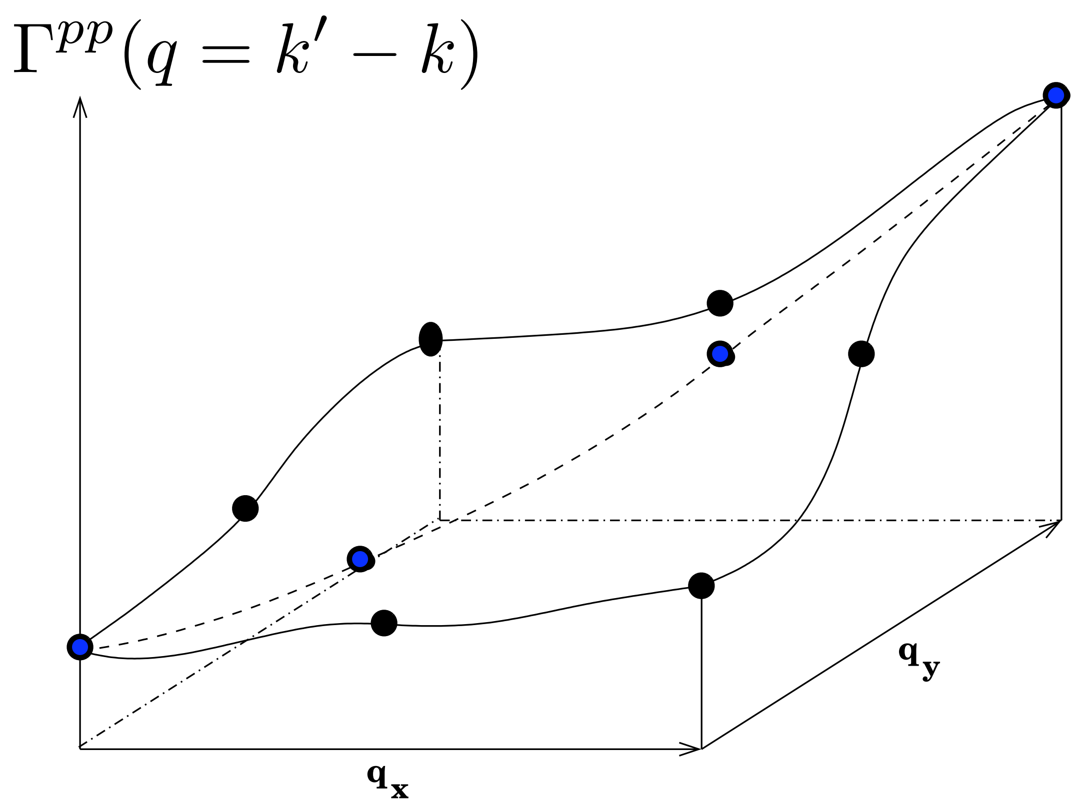


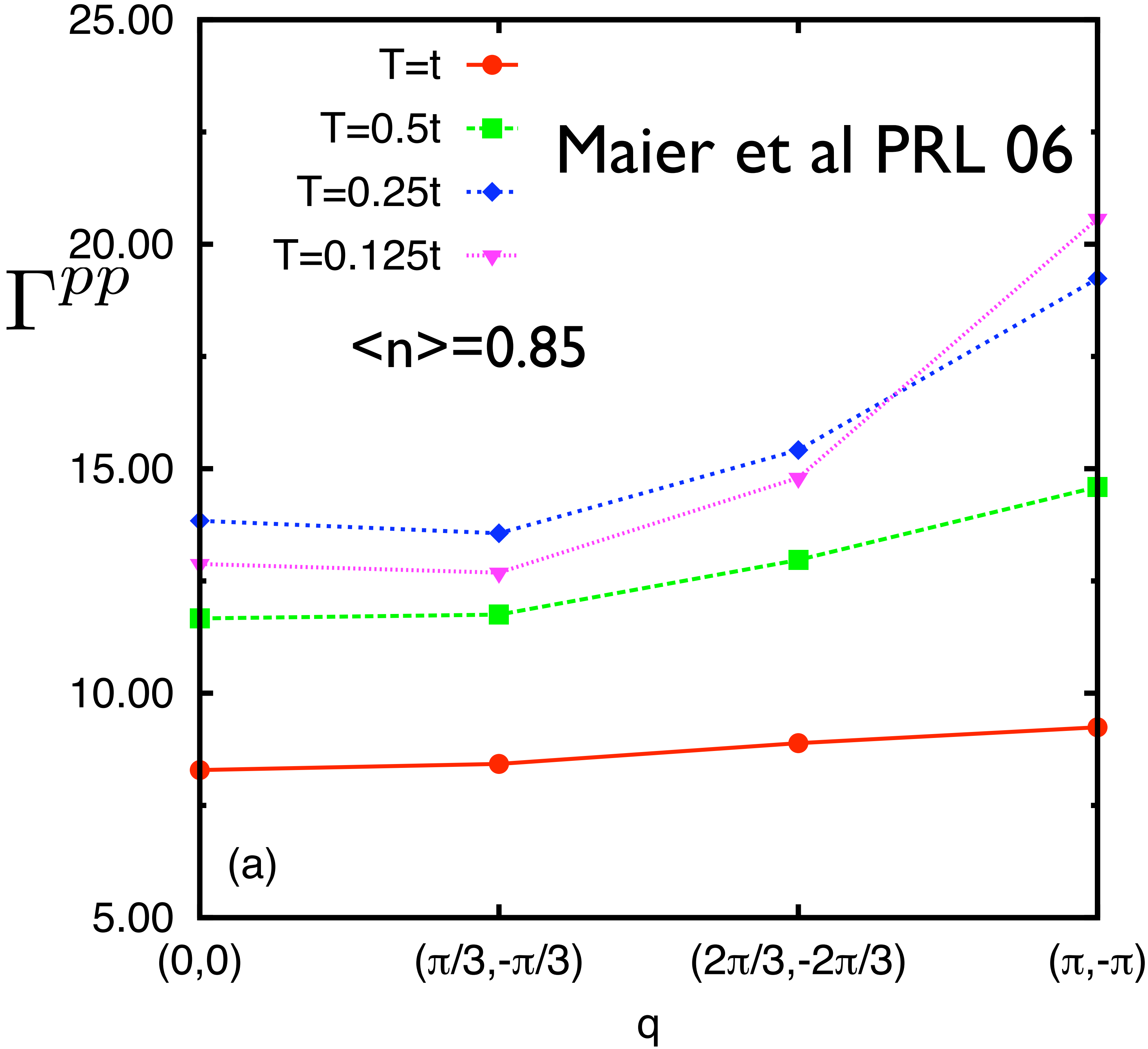
Here k=(k,iω_n). The momentum transfer is k'-k and the Matsubara energy transfer is $i\omega_{n'} - i\omega_n$.

The momentum / spatial structure of the pairing interaction

The Momentum Dependence

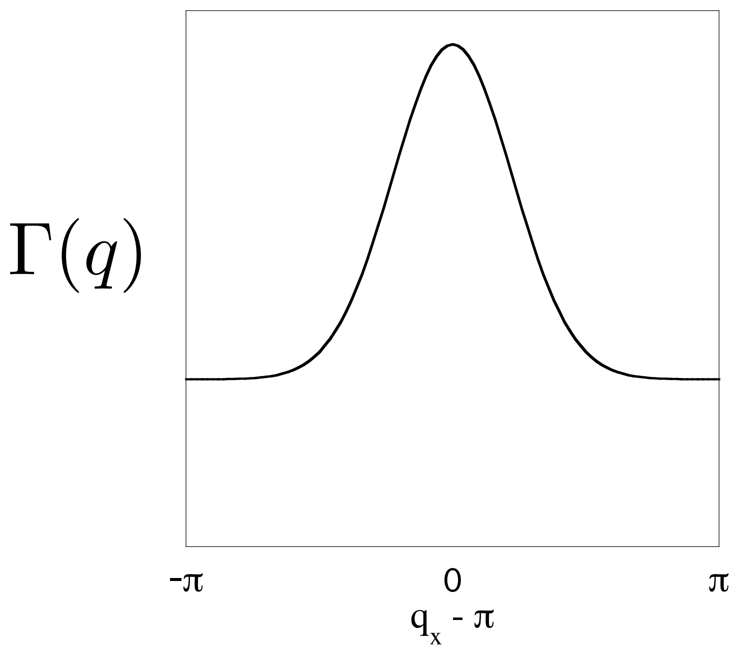
The momentum dependence of $\Gamma^{pp}(k', k)$ is shown schematically. The numerical data that I'll show is for points along qx=qy, with q=k'-k, and $\omega_n = -\omega_{n'} = \pi T$.



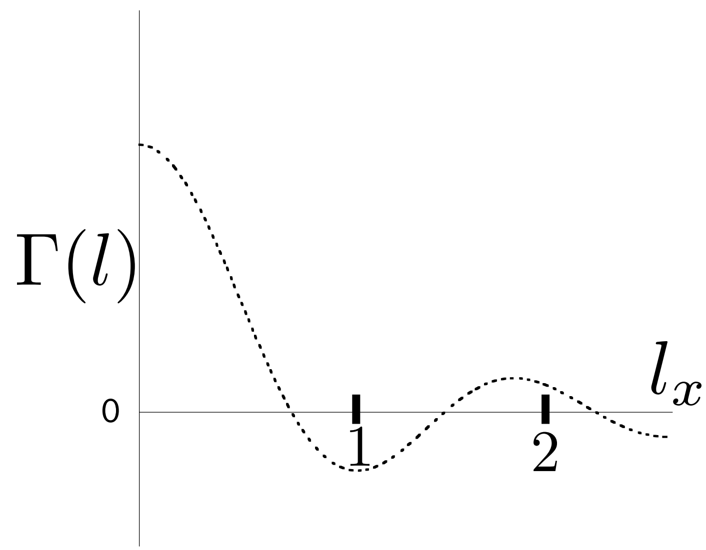

25.00
20.00
15.00
10.00
5.00
T=t
T=0.5t
T=0.25t
T=0.125t
Maier et al PRL 06
Γ^{pp}
<n>=0.85
(a)
(0,0)
(π/3,-π/3)
(2π/3,-2π/3)
(π,-π)
q

Space Dependence

The structure of the pairing interaction



Momentum Space

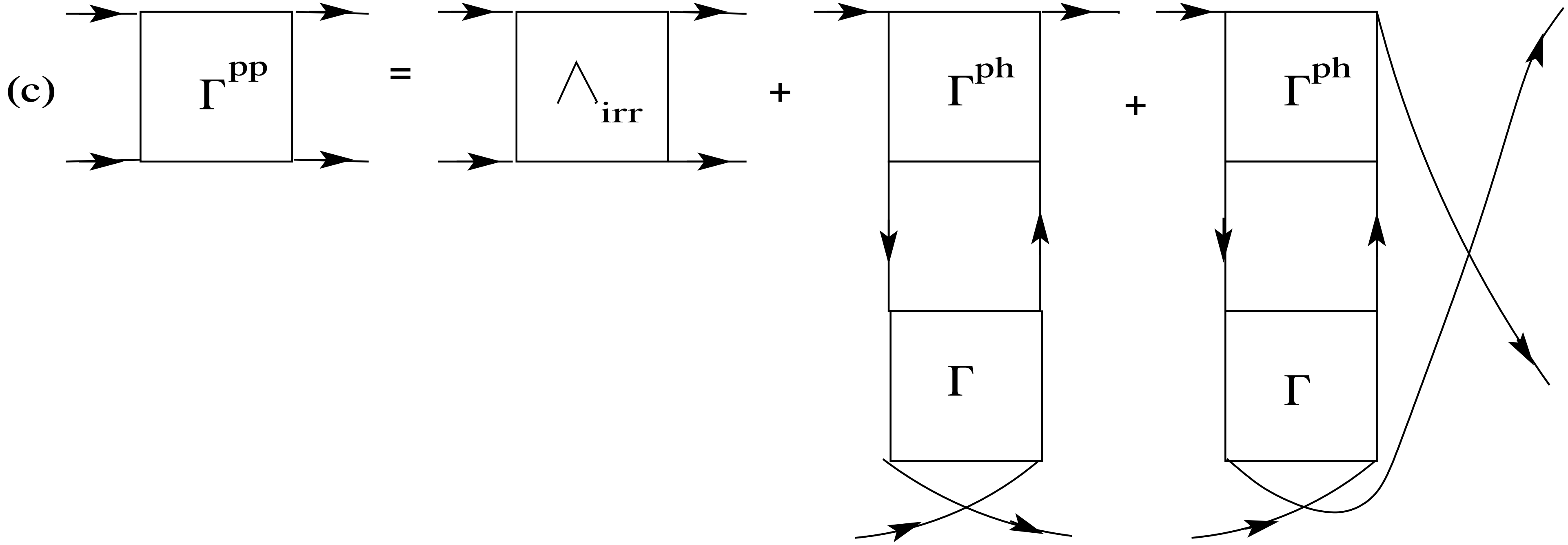


Real Space

$$\Gamma_e^{\mathrm{pp}}(\mathbf{R}) = \frac{1}{N^2} \sum_{\mathbf{p},\mathbf{p}'} e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{R}} \, \Gamma_e^{\mathrm{pp}}(\mathbf{p}', i\pi T; \mathbf{p}, i\pi T) \, .$$

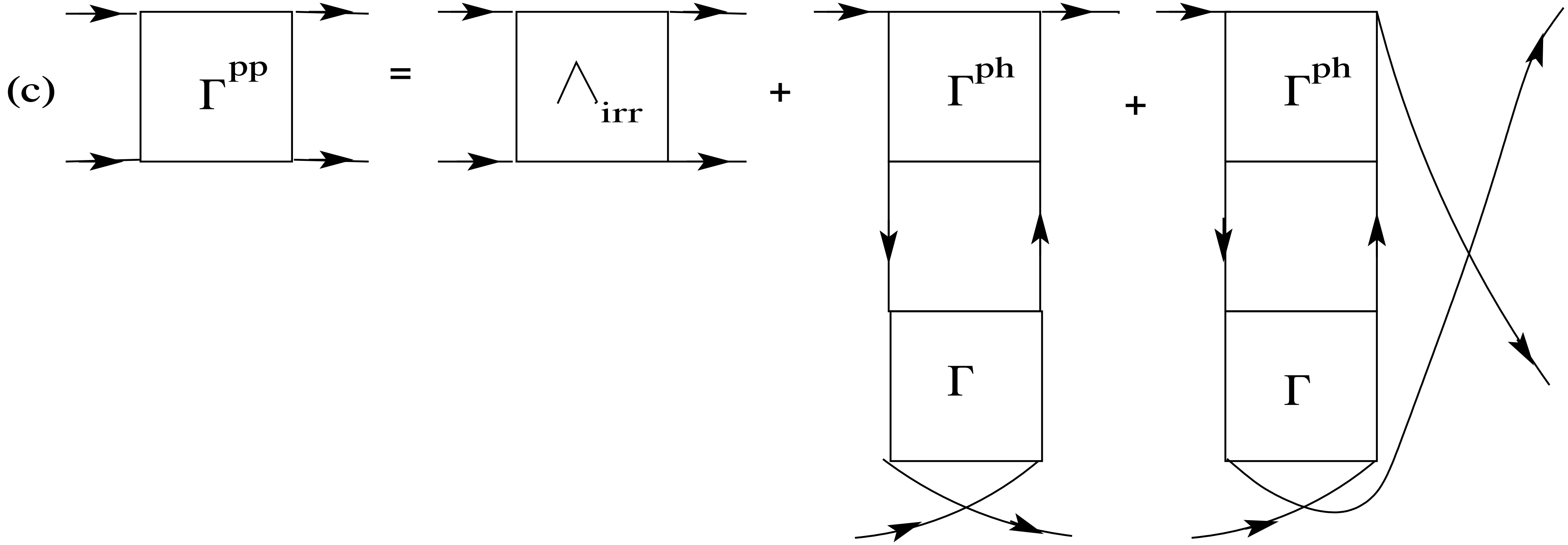
+0.01	−0.12	+0.12	−0.12	+0.01
−0.12	+0.43	−0.50	+0.43	−0.12
+0.12	−0.50	+9.6	−0.50	+0.12
−0.12	+0.43	−0.50	+0.43	−0.12
+0.01	−0.12	+0.12	−0.12	+0.01

The spin dependence of the interaction



$$\Gamma^{pp}(K,K') = \Lambda_{irr}(K,K') + \frac{1}{2}\Phi_c(K,K') + \frac{3}{2}\Phi_m(K,K')$$

(Pfitzner, Wölfle, PRB ‘89; Esirgen, Bickers, PRB ‘98)

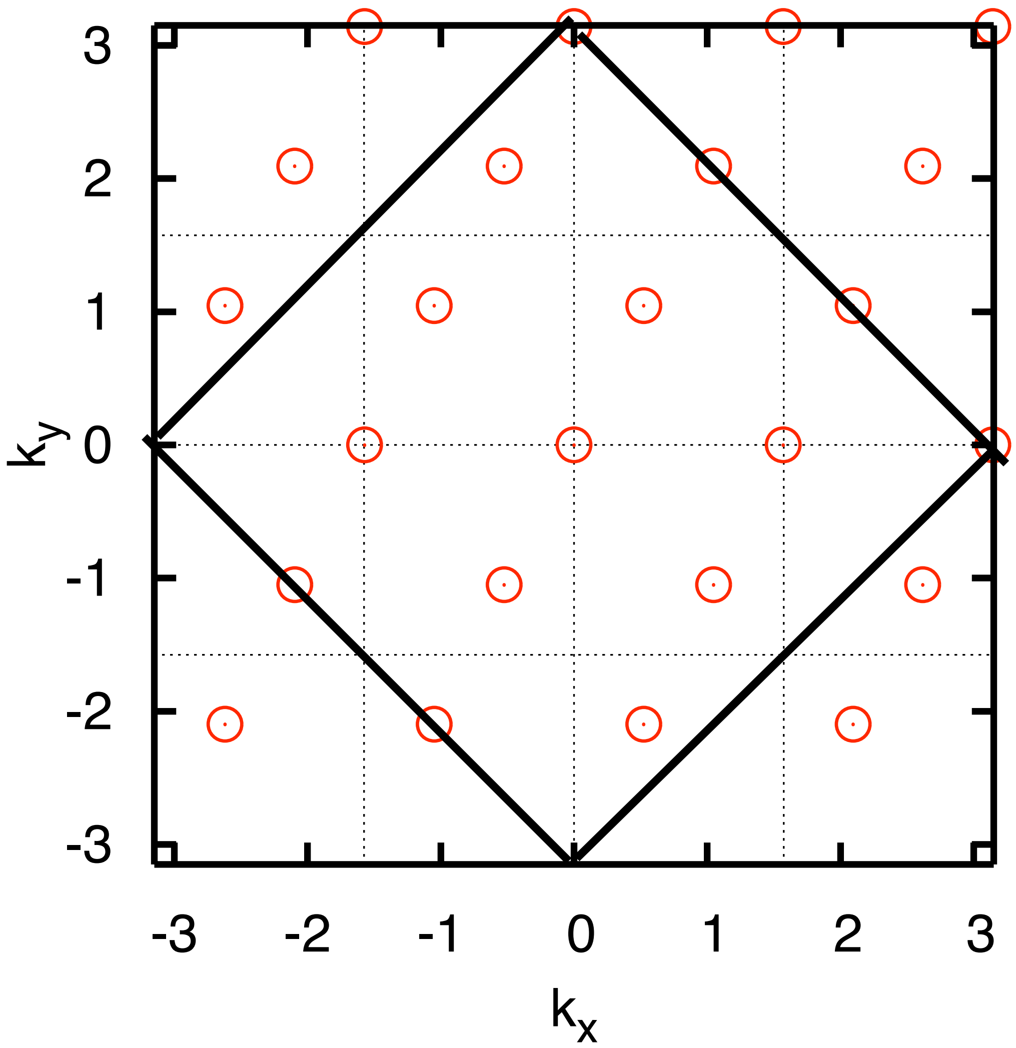


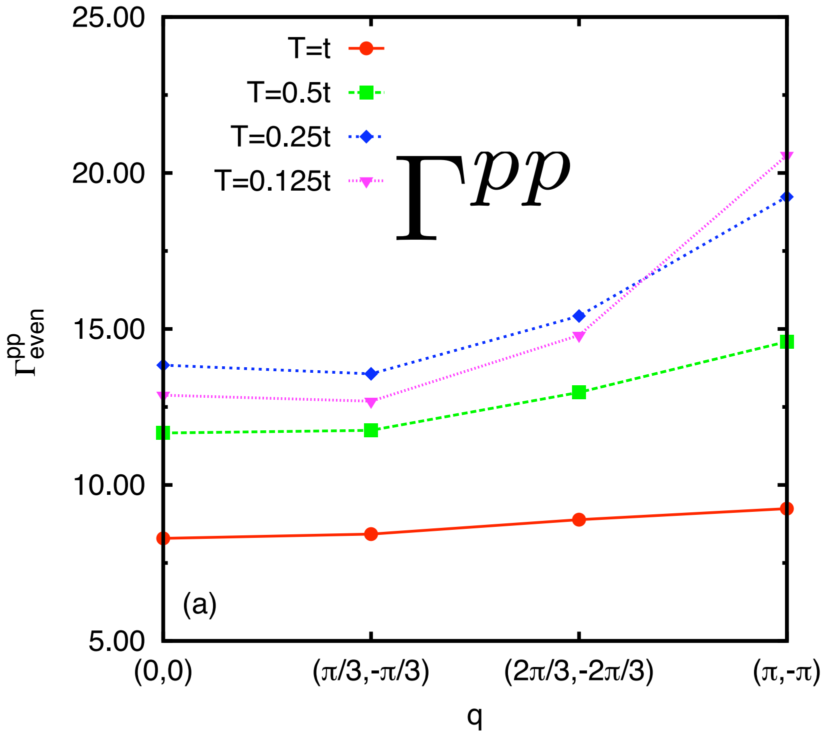
$$\Gamma^{pp}(K,K') = \Lambda_{irr}(K,K') + \frac{1}{2}\Phi_c\,(K,K') + \frac{3}{2}\Phi_m(K,K')$$

S=0 S=1

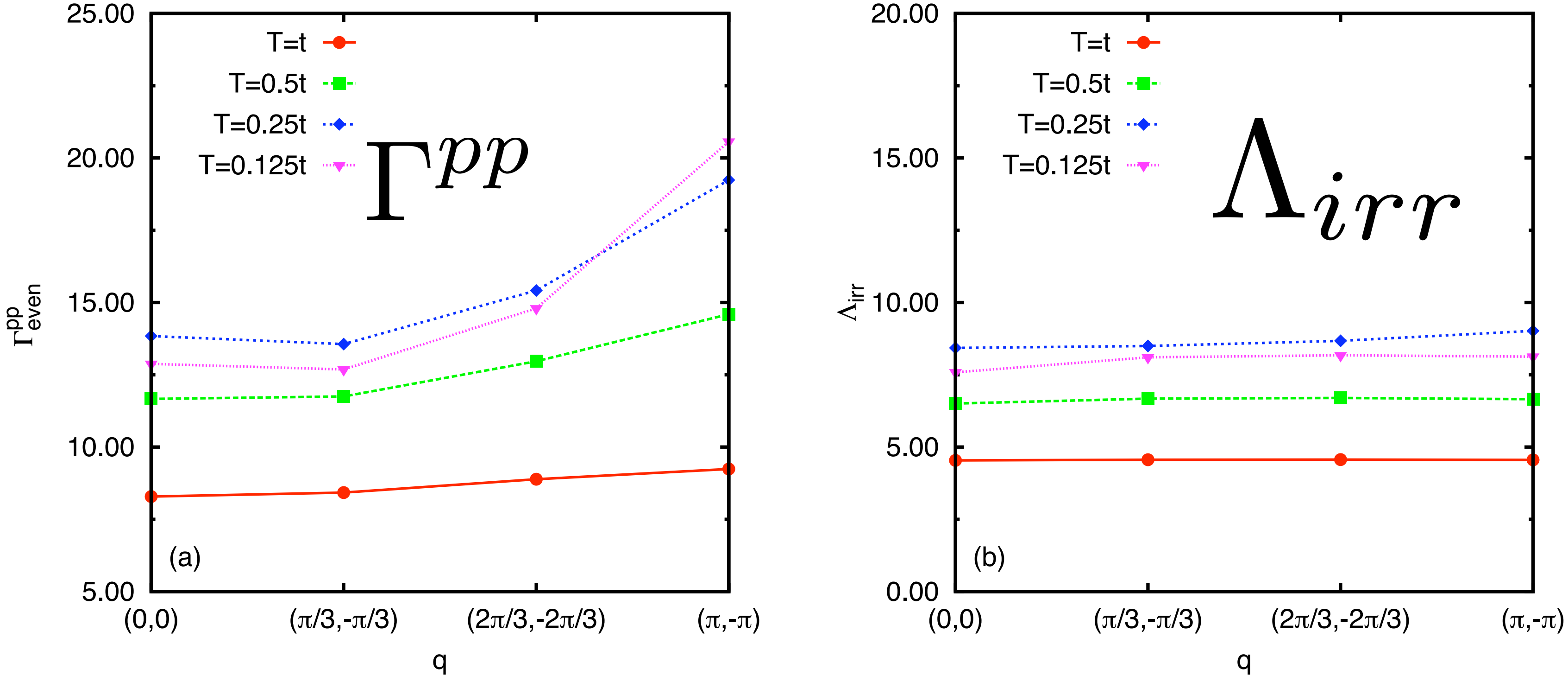
(Pfitzner, Wölfle, PRB '89; Esirgen, Bickers, PRB '98)

Cluster k-points

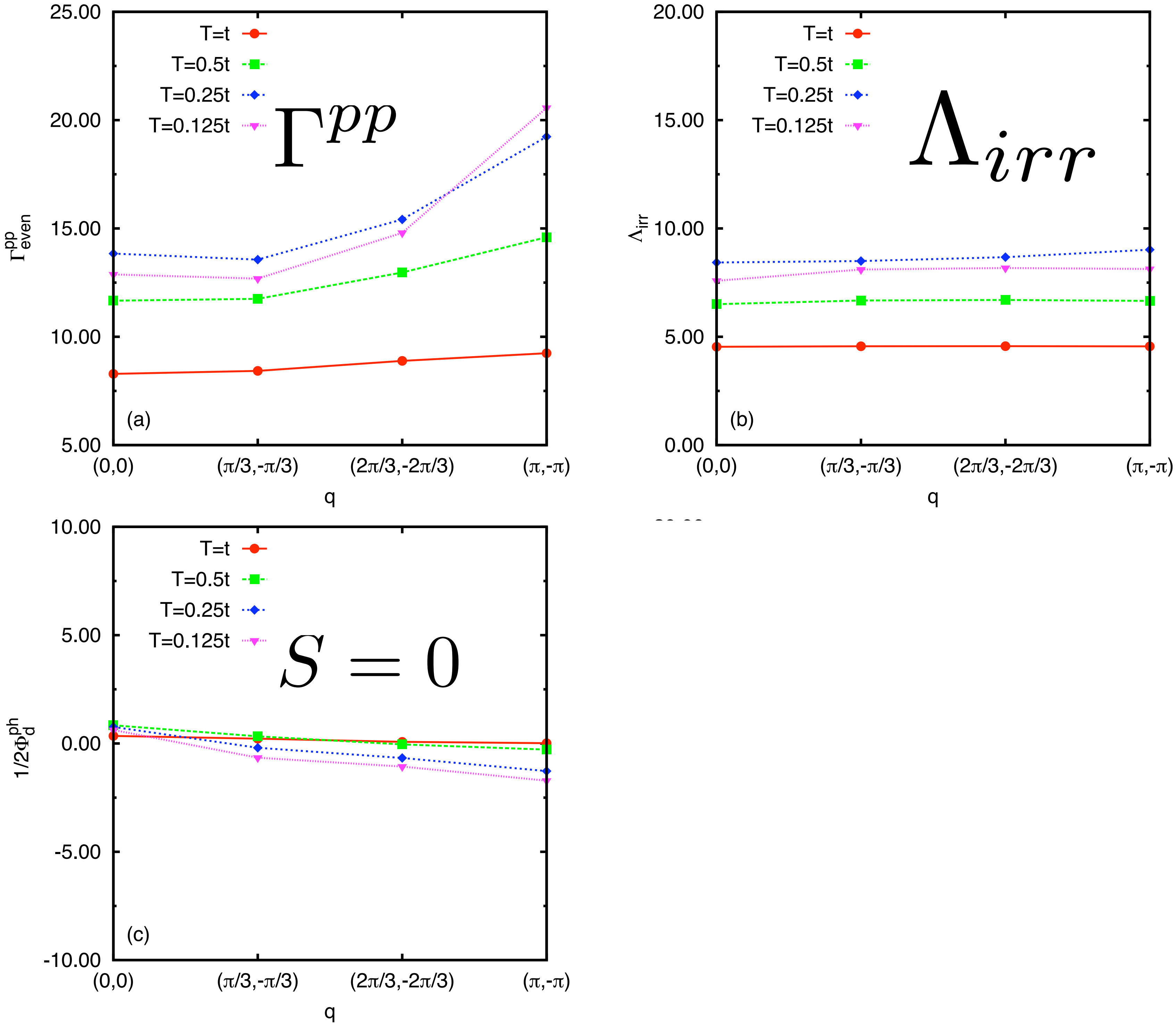




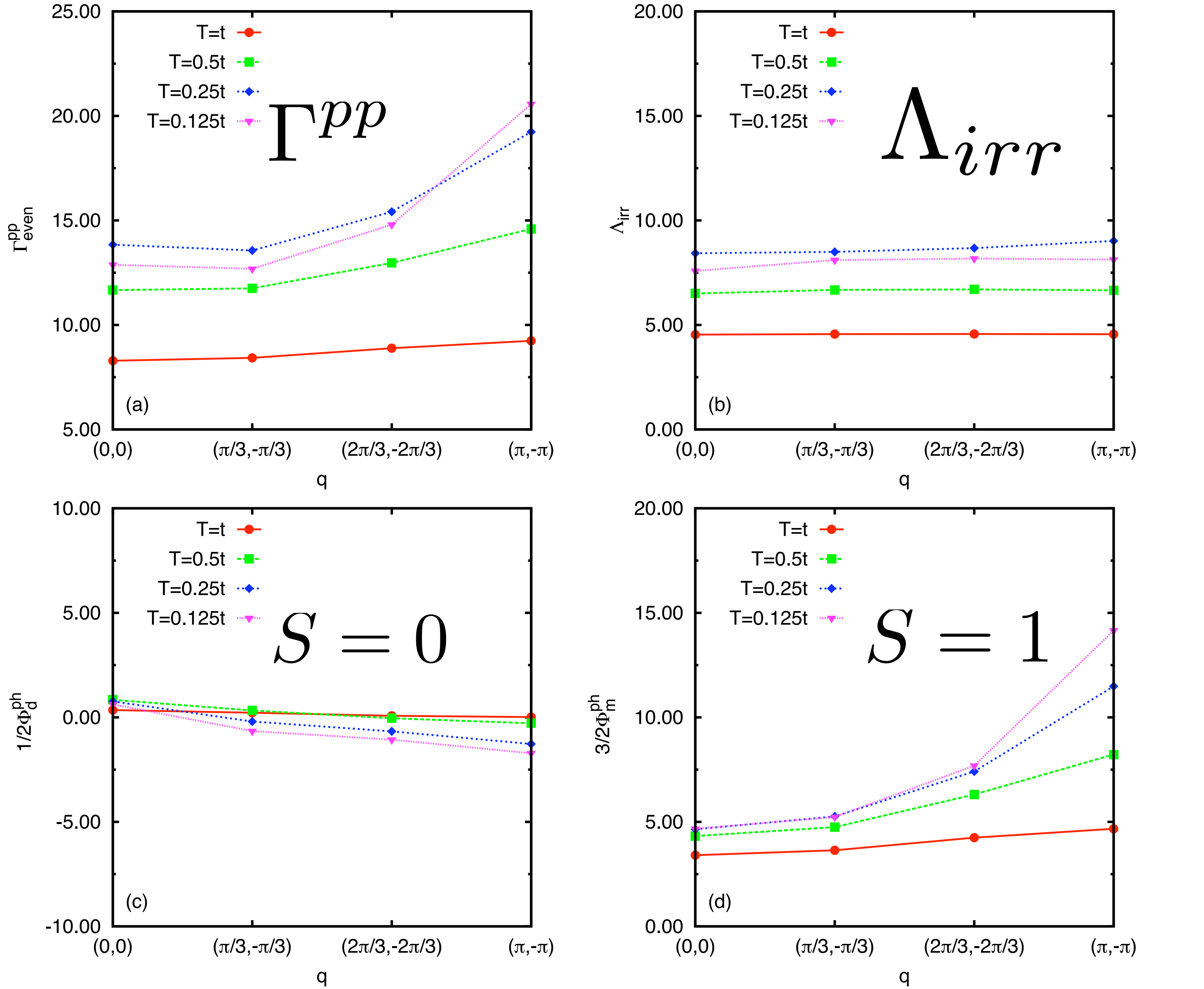
Maier et al PRL 06



Maier et al PRL 06



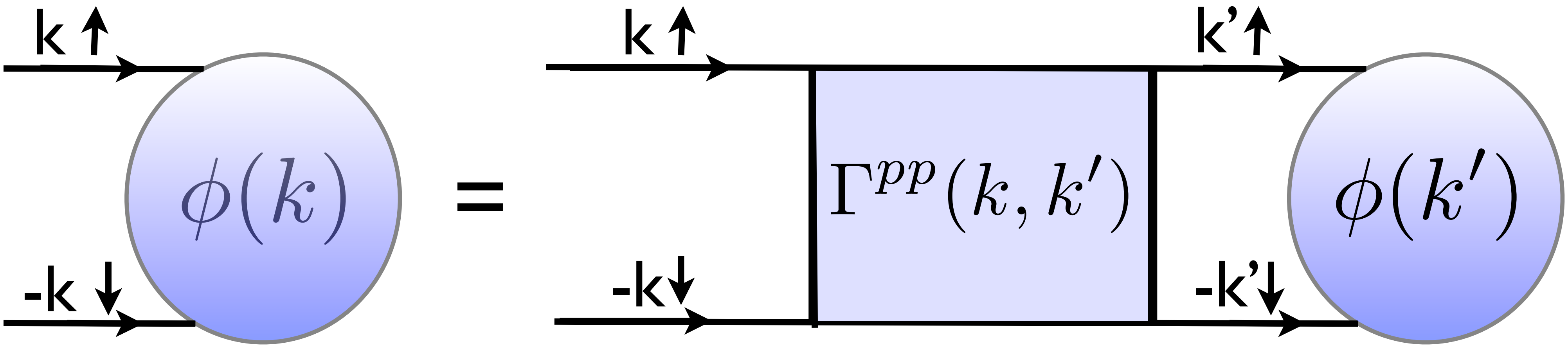
Maier et al PRL 06



Maier et al PRL 06

There is another way to discuss the structure of the pairing interaction.

The Bethe-Salpeter equation in the pairing channel is



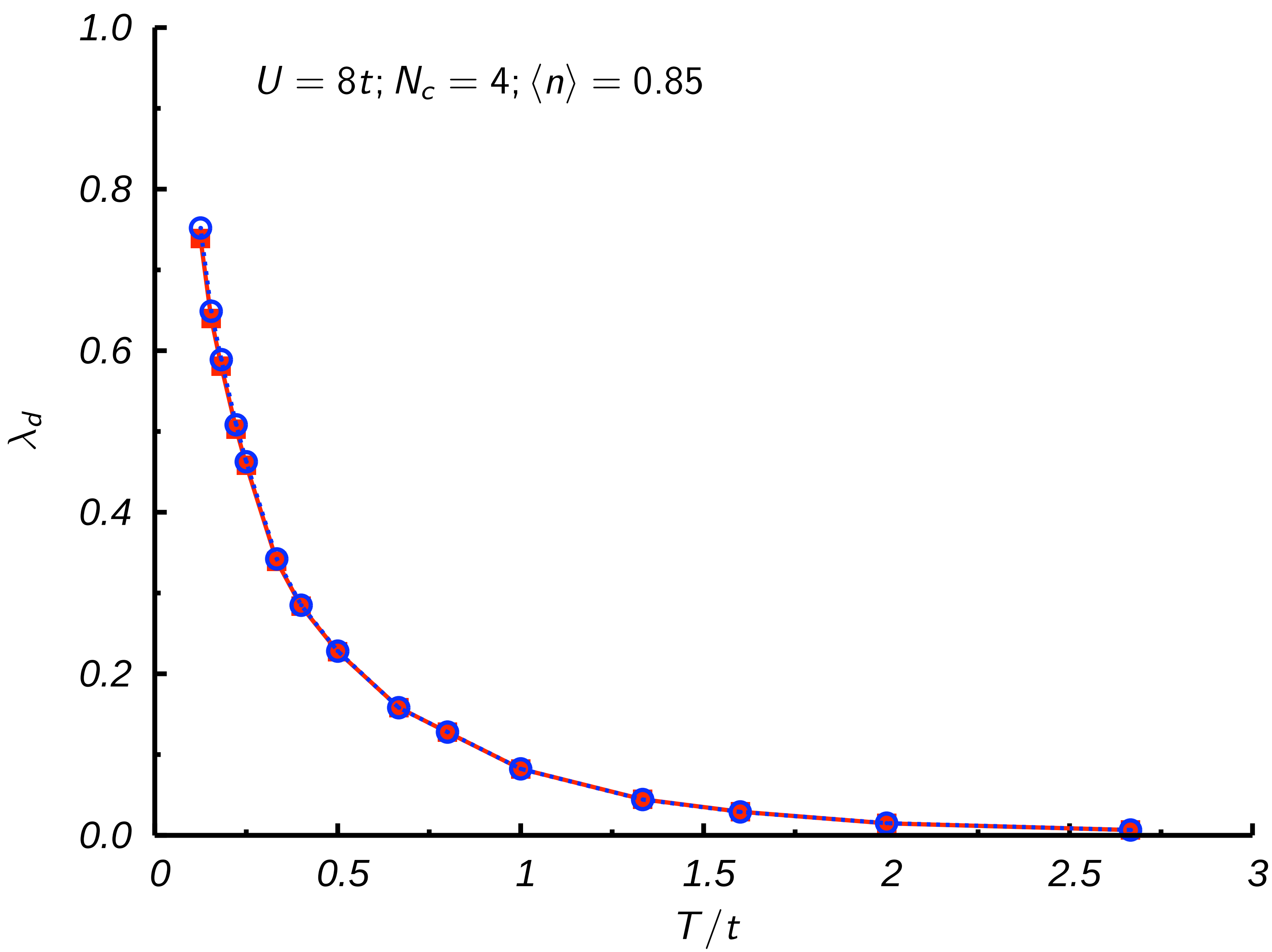
$$k = (\mathbf{k}, i\omega_n)$$

There is another way to discuss the structure of the pairing interaction.

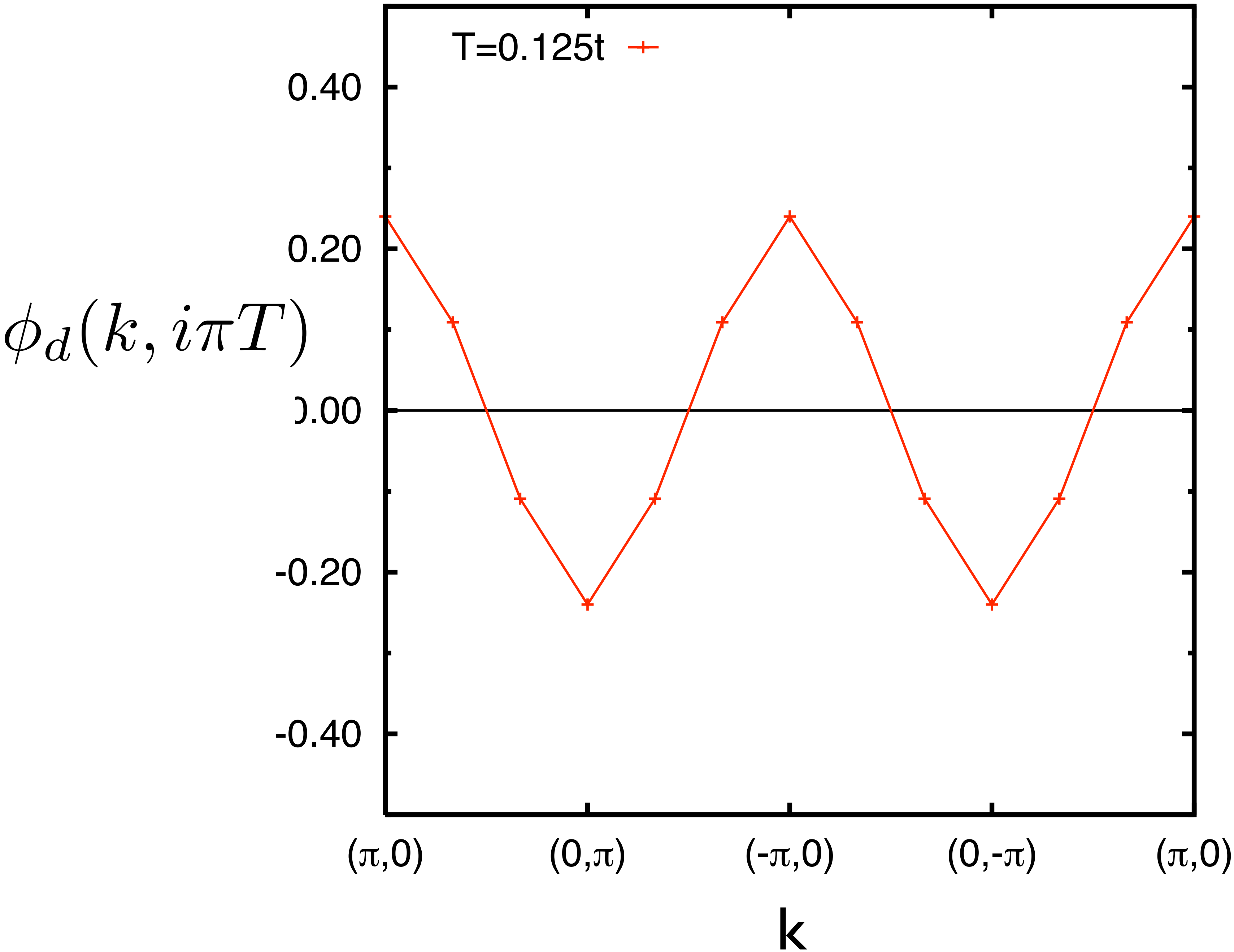
The Bethe-Salpeter equation in the pairing channel is

$$-(T/N)\sum_{k'}\Gamma^{pp}(k,k')G(k')G(-k')\phi_\alpha(k') = \lambda_\alpha\phi_\alpha(k)$$

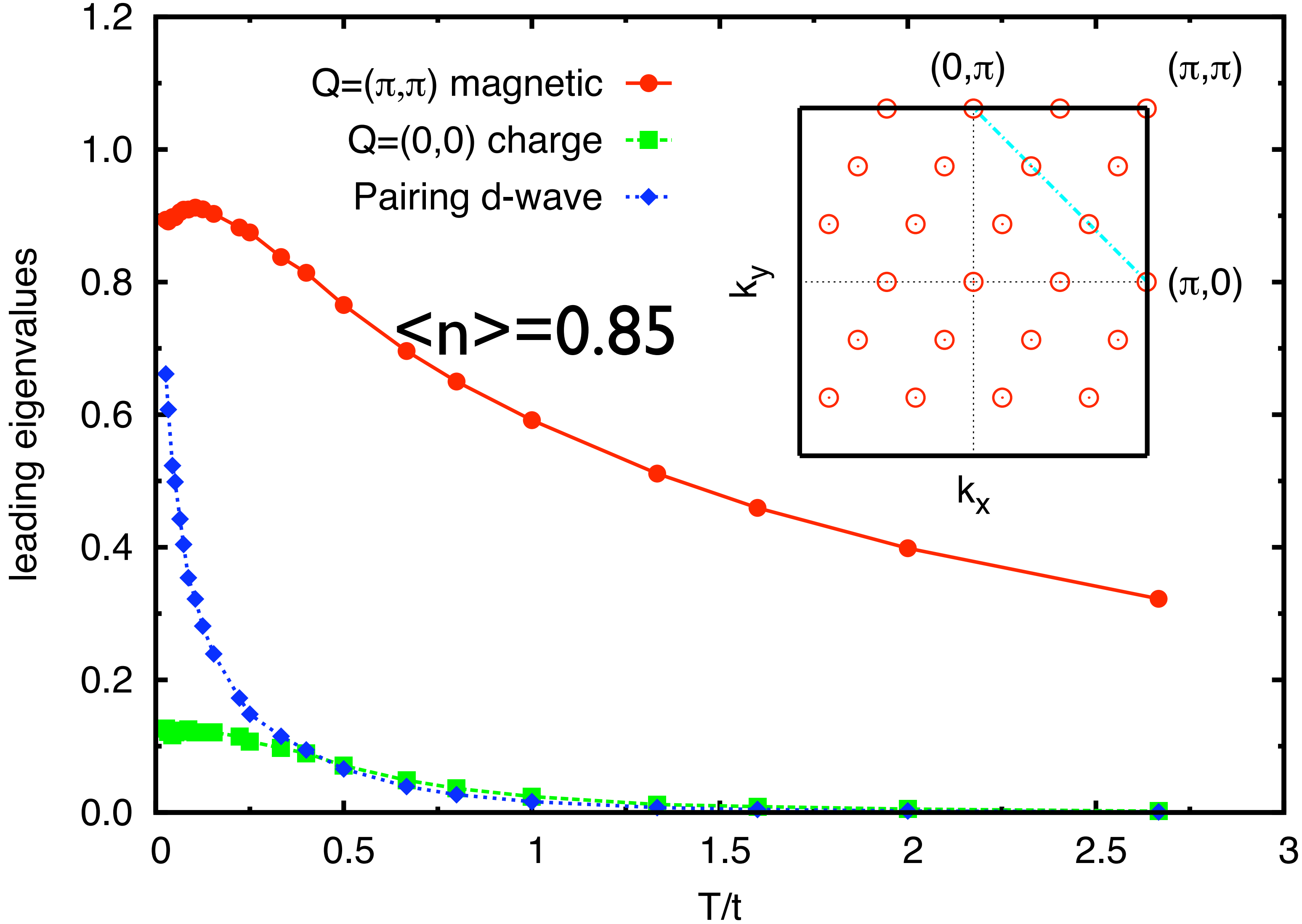
$$k = (\mathbf{k}, i\omega_n)$$



$U = 8t; N_c = 4; \langle n \rangle = 0.85$
1.0
0.8
0.6
0.4
0.2
0.0
λ_d
0
0.5
1
1.5
2
2.5
3
T/t

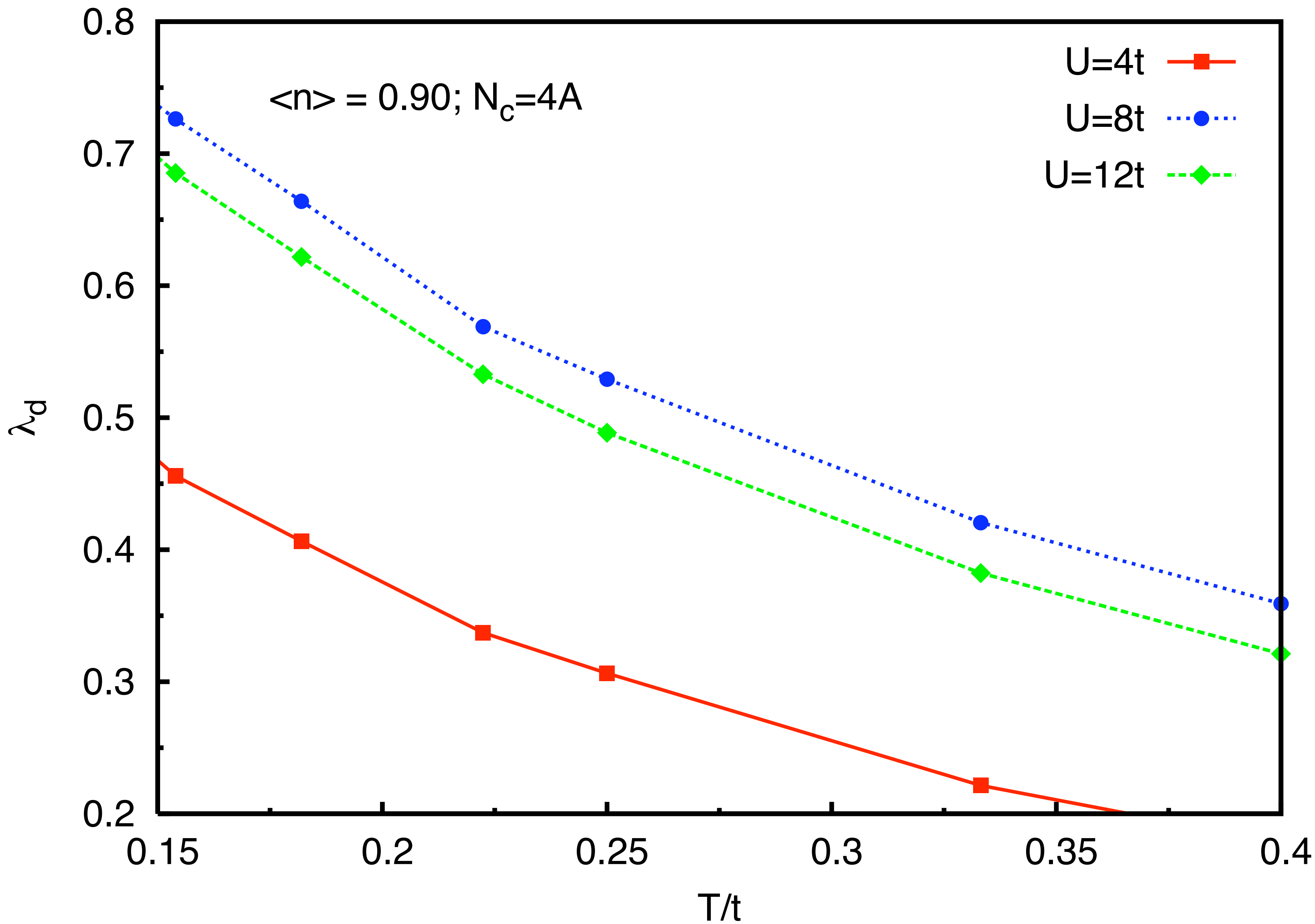

T=0.125t
0.40
0.20
0.00
-0.20
-0.40
$\phi_d(k, i\pi T)$
(π,0)
(0,π)
(-π,0)
(0,-π)
(π,0)
k

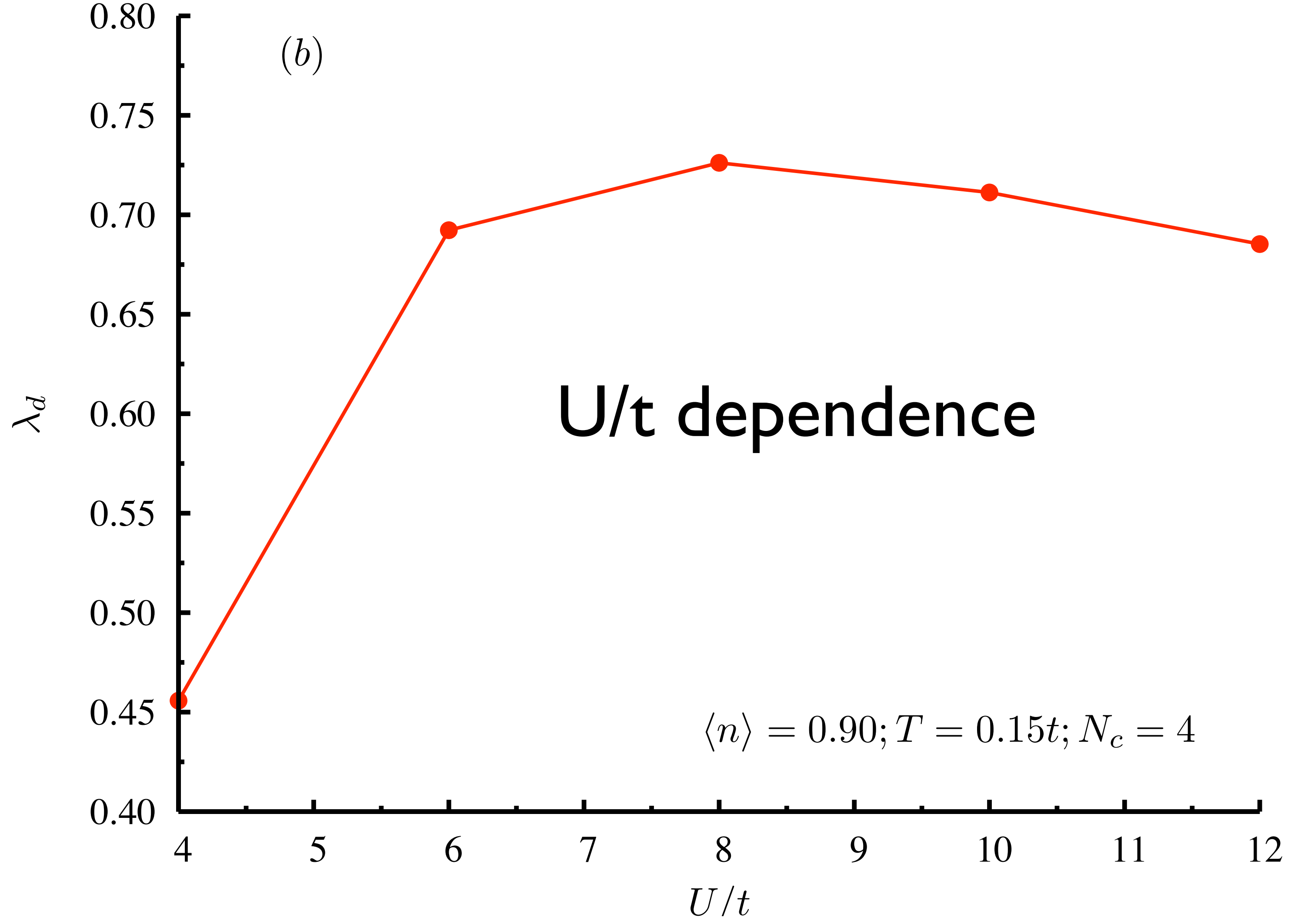
Leading eigenvalues



Coupling strength U/t dependence

Coupling strength dependence

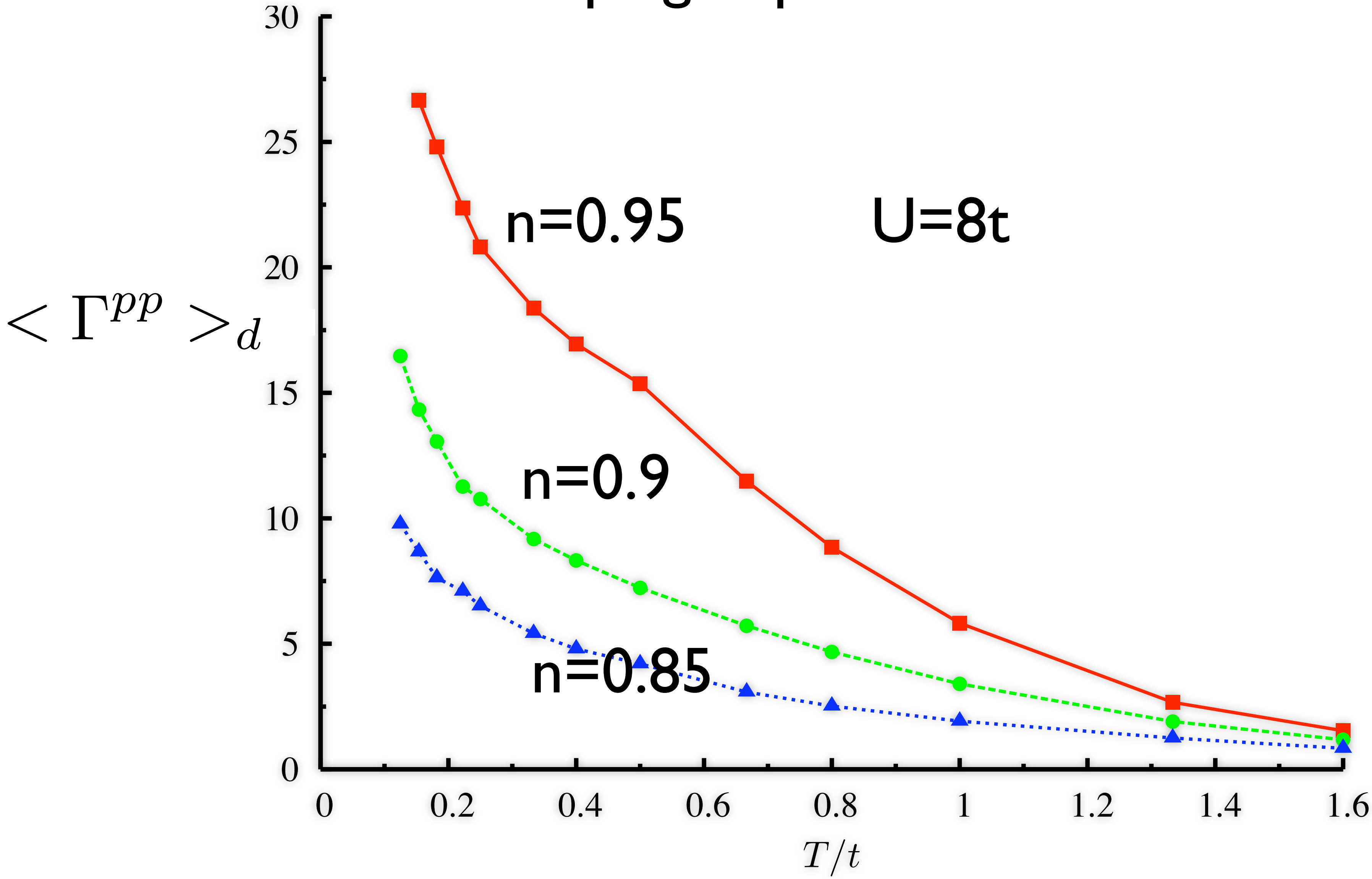




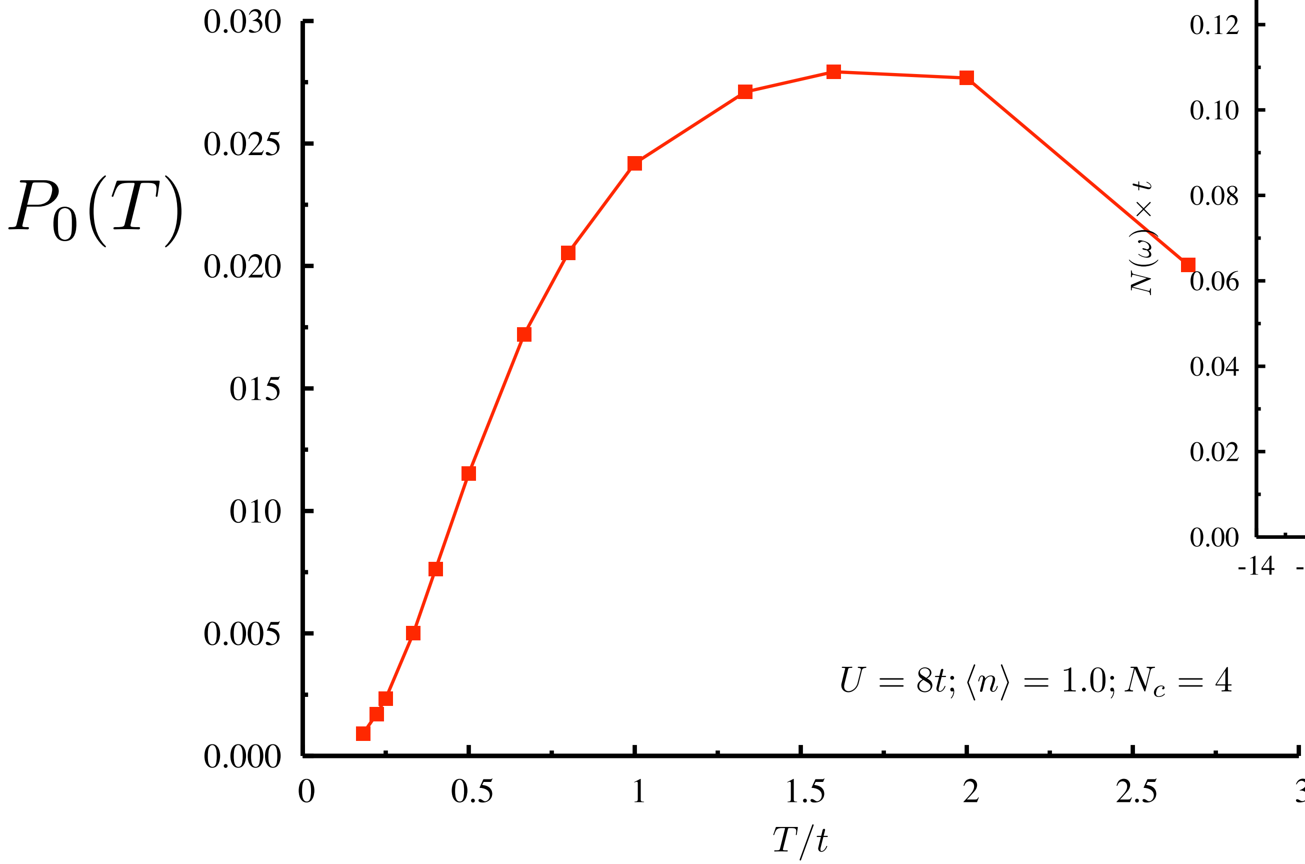
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
(b)
λ_d
U/t dependence
$\langle n \rangle = 0.90; T = 0.15t; N_c = 4$
4
5
6
7
8
9
10
11
12
U/t

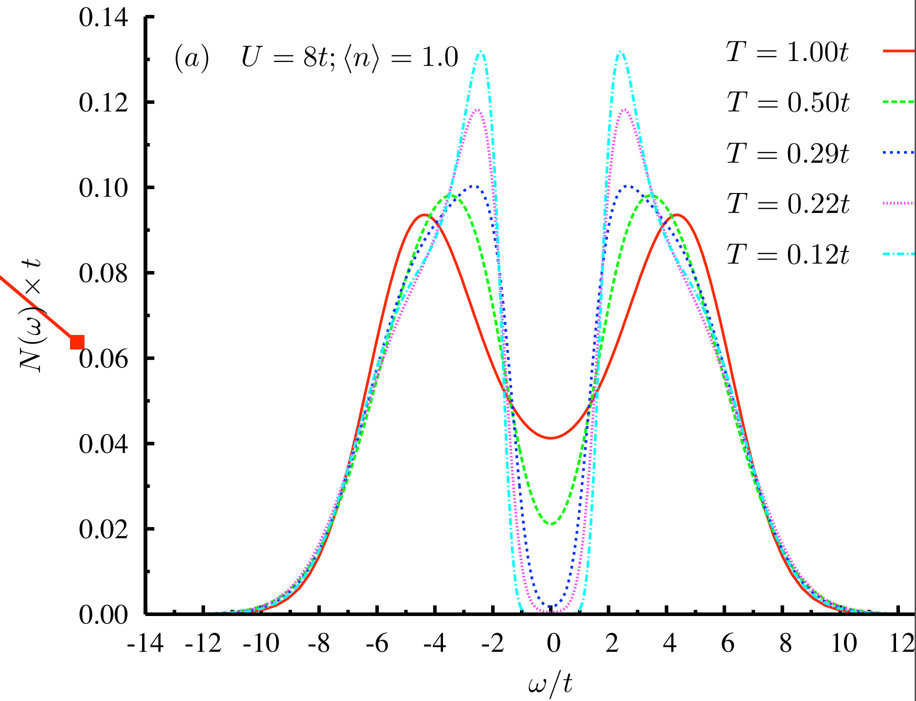
The doping dependence

Doping dependence



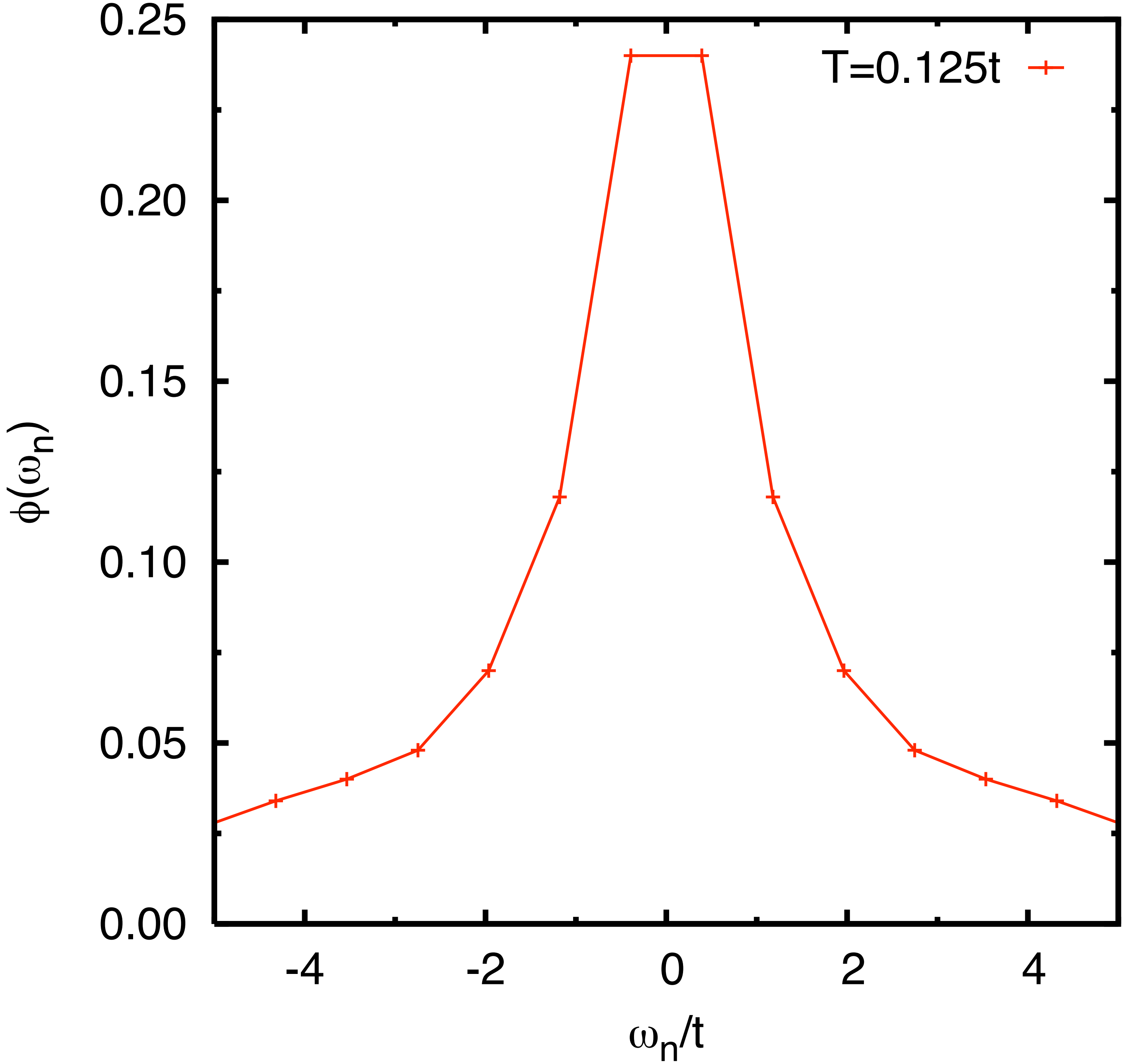
$$P_0(T) = \frac{T}{N}\sum_K (cosk_x - cosk_y)^2 G_\uparrow(K) G_\downarrow(-K)$$



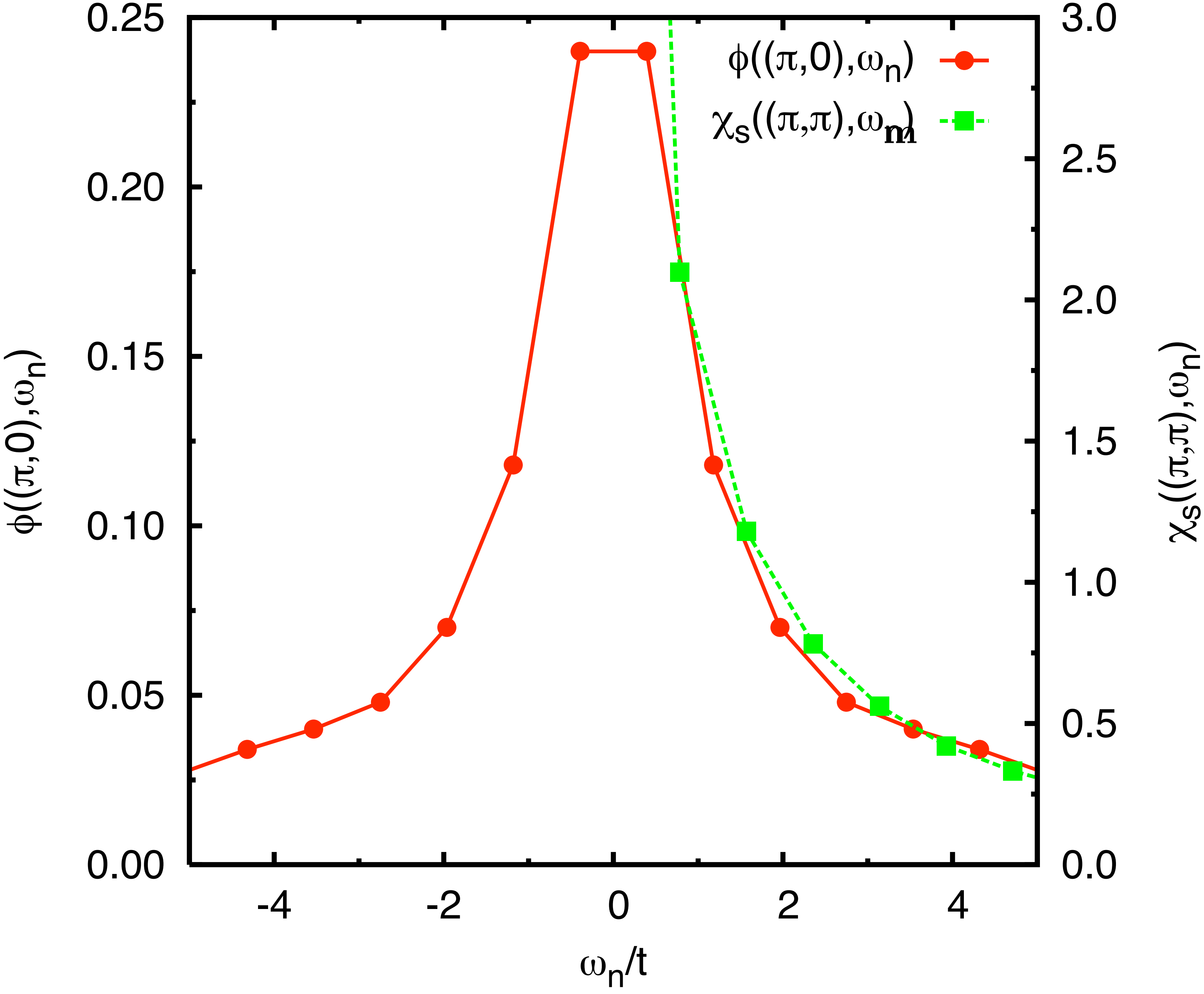


The frequency dependence and the question of Glue.

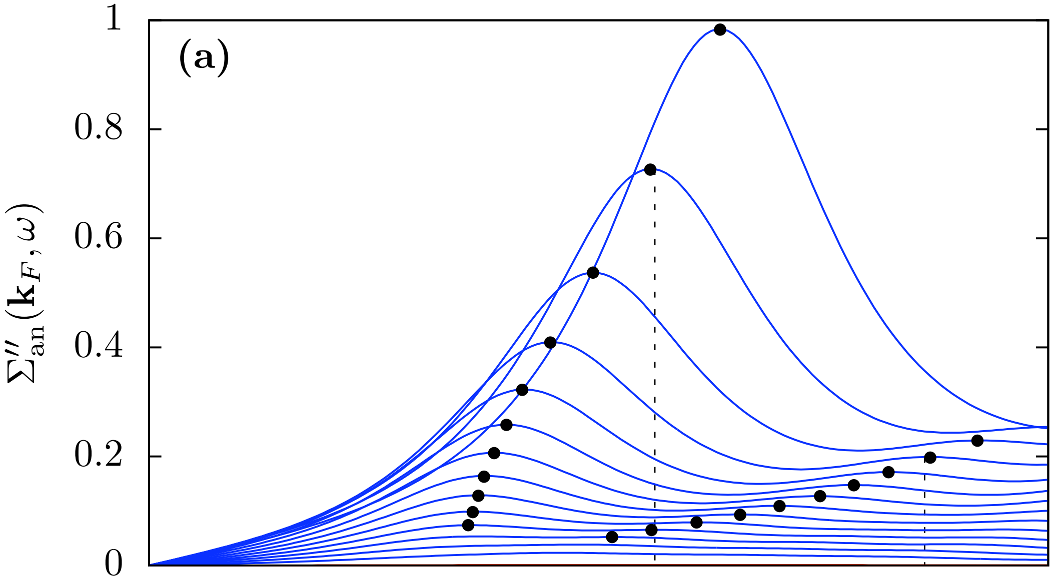
The dynamics is characterized by the frequency dependence of the gap function. Here we look at the Matsubara $i\omega_n$ dependence of $\phi_d(k, i\omega_n)$



0.25
0.20
0.15
0.10
0.05
0.00
-4
-2
0
2
4
φ(ωn)
ωn/t
T=0.125t



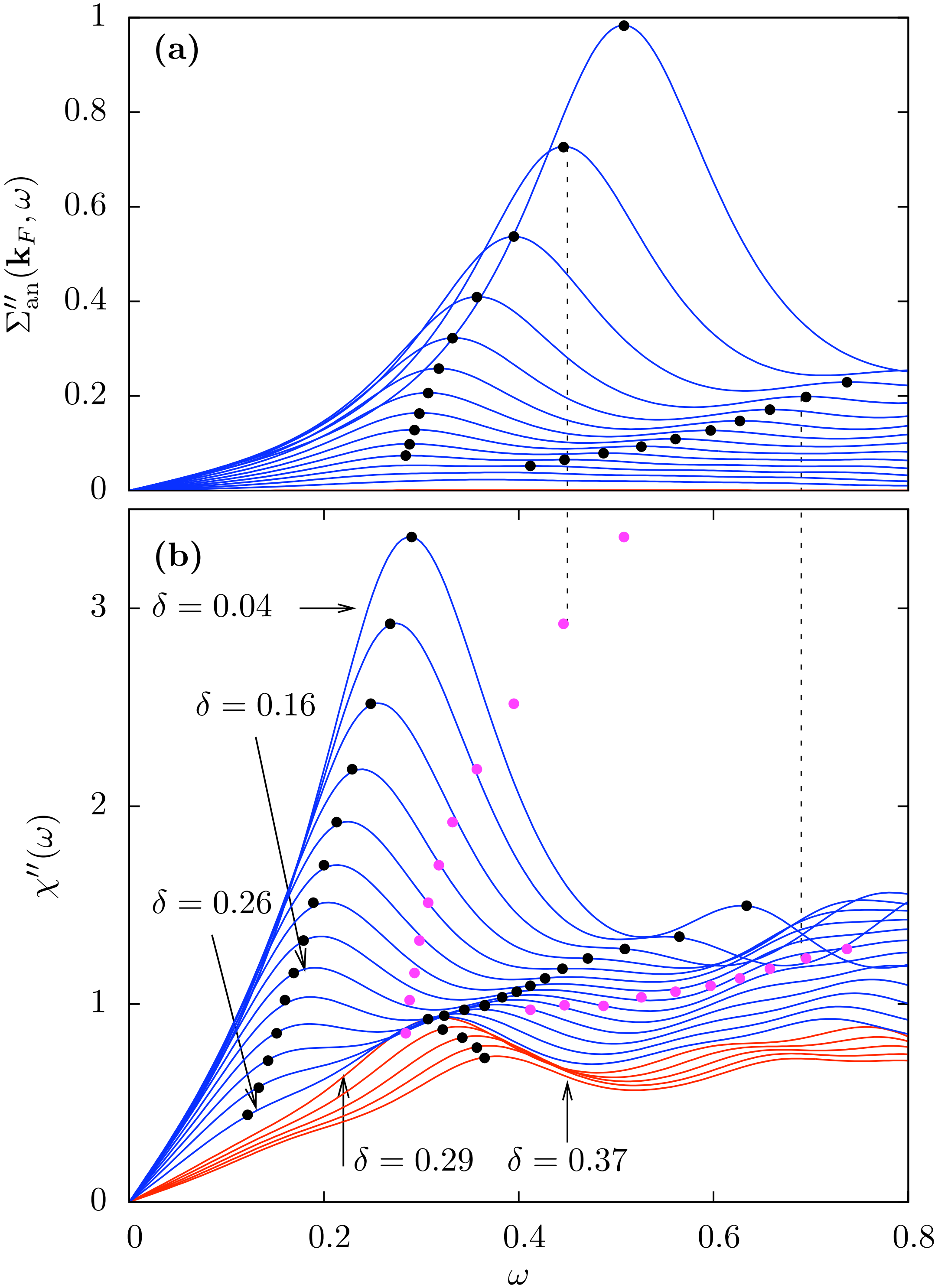
0.25
0.20
0.15
0.10
0.05
0.00
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-4
-2
0
2
4
ω_n/t
$\phi((\pi,0),\omega_n)$
$\chi_s((\pi,\pi),\omega_n)$
$\phi((\pi,0),\omega_n)$
$\chi_s((\pi,\pi),\omega_m)$



B. Kyung, D. Senechal and A.-M. Tremblay arXiv 0812.1228

t’=-0.17t t”=0.08
U=8t

C-DMFT



B. Kyung, D. Senechal and A.-M. Tremblay arXiv 0812.1228

t'=-0.17t t''=0.08
U=8t

C-DMFT

The effective pairing interaction for the 2D hubbard model:

* increases at large momentum transfers leading to an attractive near neighbor d-wave pairing
* is dominantly carried by a spin S=1 particle-hole channel
* is largest for U~8t
* increases as n goes towards 1.
* is retarded on a scale set by the dynamic spin susceptibility

Comments on Mike Norman's Questions

There is pairing Glue in the Hubbard model and it reflects pairing that is mediated by spin-fluctuations. The same electrons that make up the pairs provide the the spin-fluctuations that mediate the pairing. This is why the coupling to the "glue" is strong.

Comments on Mike Norman's Questions

There is pairing Glue in the Hubbard model and it reflects pairing that is mediated by spin-fluctuations. The same electrons that make up the pairs provide the the spin-fluctuations that mediate the pairing. This is why the coupling to the "glue" is strong.

This is important because it implies that in thinking about the pairing interaction in Hubbard like models one should focus on the proximity to anti-ferromagnetism and the spin-fluctuations spectrum.

Comments on Mike Norman's Questions

There is pairing Glue in the Hubbard model and it reflects pairing that is mediated by spin-fluctuations. The same electrons that make up the pairs provide the the spin-fluctuations that mediate the pairing. This is why the coupling to the "glue" is strong.

This is important because it implies that in thinking about the pairing interaction in Hubbard like models one should focus on the proximity to anti-ferromagnetism and the spin-fluctuations spectrum.

Spin-fluctuations provide a unified framework for thinking about pairing in the heavy fermions, the actinides, the cuprates and the Fe-pnictides.

There will be spectroscopic signatures of $\chi''(k,\omega)$ in the frequency dependence of $\Delta(k,\omega)$.

These signatures appear in tunneling, optical and ARPES experiments, but in the absence of a small parameter and the occurrence of other phenomena, they are more difficult to extract than the phonon signatures in the traditional low Tc superconductors.

Collective modes

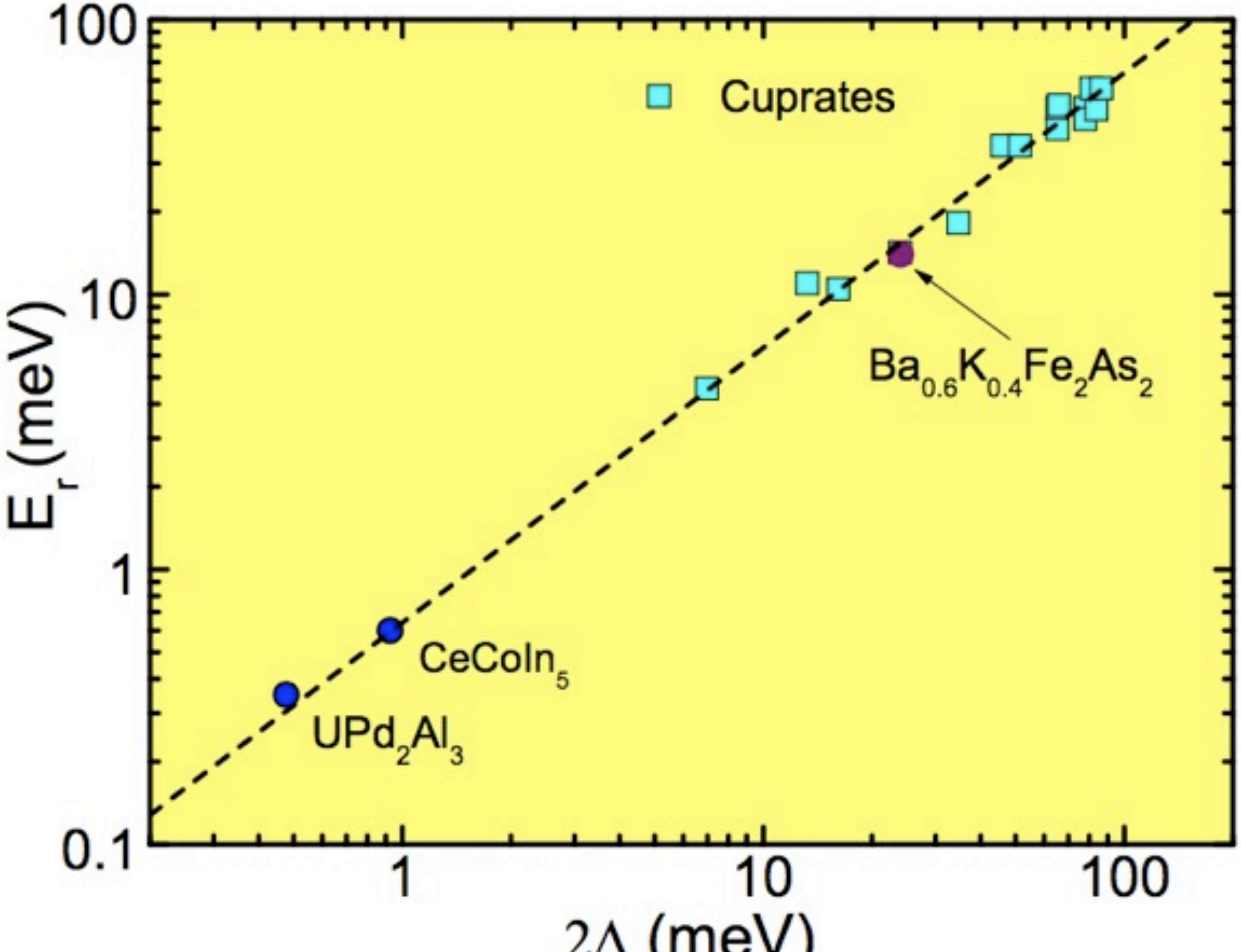
The occurrence of the neutron scattering pi-resonance arises naturally in a FLEX treatment of the Hubbard model. In general it tells one that

$$\Delta(k+Q) = -\Delta(k)$$

with Q the wave vector of the resonance.

I believe that a gap which changes sign suggests that the pairing is mediated by an electron-electron interaction.

A.Christianson et al
0807.3932



There is a possibility of a collective Bardasis-Schrieffer excitonic mode in the Fe superconductors.

Spin-fluctuation calculations for the Fe superconductors find an attractive pairing interaction in both the A_{1g} (s-wave) and B_{1g} (d-wave) channels. This raises the possibility that a Bardasis-Schrieffer collective excitonic mode is present which may be seen in Raman scattering.

W.-C. Lee, S.-C. Zhang, and C. Wu 0810.1309
D. Scalapino and T. Devereau 0904.1973