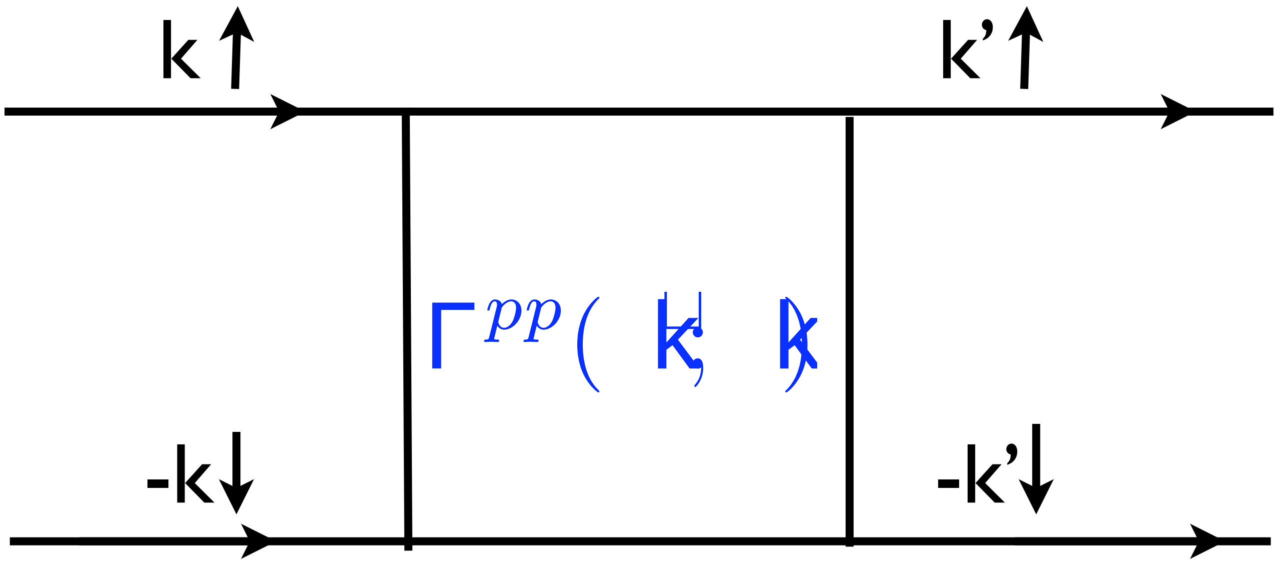
The Structure of the Pairing Interaction in the 2D Hubbard model

Mark Jarrell (UC),Thomas Maier(ORNL),DJS(UCSB)

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

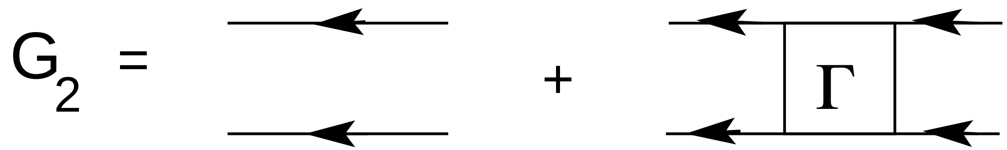


Here k=(k,i ω_n). The momentum transfer is k-k' and the Matsubara energy transfer is $i\omega_n - i\omega_{n'}$.

In the quantum Monte Carlo frame work one calculates finite temperature Green's functions. In order to calculate the pairing interaction we have calculated the one and two particle Green's functions:

$$G(2,1) = -< T c_{p_2}(\tau_2) c_{p_1}^{\dagger}(\tau_1) >$$

$$G_2(4,3,2,1) = - < T c_{p_4}(\tau_4) c_{p_3}(\tau_3) c_{p_2}^{\dagger}(\tau_2) c_{p_1}^{\dagger}(\tau_1) >$$



$$\mathbf{G_2(p', k'; k, p) = -\boldsymbol{\delta}_{p'p}\boldsymbol{\delta}_{k'k}\ G_{\uparrow}(p)\, G_{\downarrow}(k)}$$

$$\mathbf{+\frac{T}{N}\,\boldsymbol{\delta}_{k'+p'-k-p}\ G_{\uparrow}(p')\, G_{\downarrow}(k')\Gamma(p', k'; k, p)\ G_{\uparrow}(p)\, G_{\downarrow}(k)}$$

$$\mathbf{\Gamma(p', k'; k, p) \sim \frac{G_2(p', k'; k, p)}{G(p')\, G(k')\, G(k)\, G(p)}}$$

Once we have calculate the full vertex

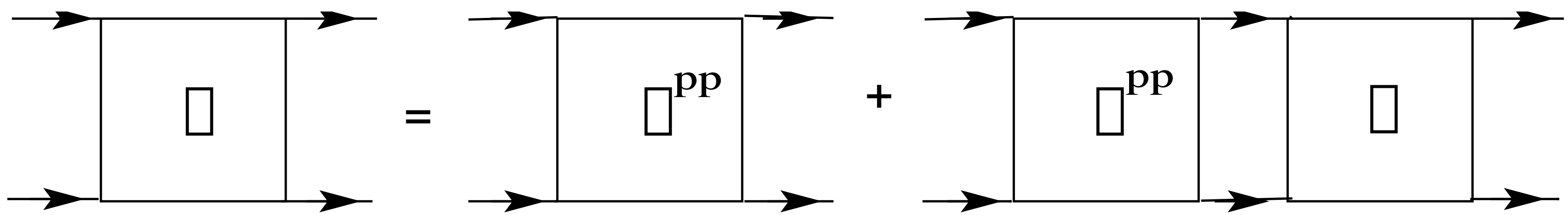
$\Gamma\ (p, k, p', k'))andG(p)$ then we can determine Γ^{pp}.

This is the opposite of what one usually does, when one selects some subset of diagrams to approximate the irreducible vertex and then sets out to calculate the full vertex.

Here we use the Monte Carlo to determine the full vertex and then solve the usual t-matrix equation "backwards" to find the irreducible vertex.

The irreducible particle-particle vertex Γ^{pp}

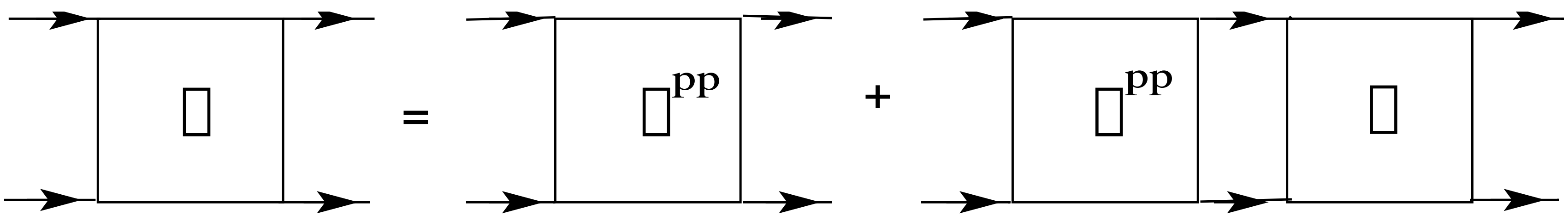
(a)



$$\Gamma(p;p') = \Gamma^{pp}(p;p'') + (T/N)\sum_{p''}\Gamma^{pp}(p;p'')G(p'')G(-p'')\Gamma(p'';p')$$

The irreducible particle-particle vertex Γ^{pp}

(a)



$$\Gamma(p;p') = \Gamma^{pp}(p;p'')$$

$$+(T/N)\sum_{p''}\Gamma^{pp}(p;p'')G(p'')G(-p")\Gamma(p";p')$$

Now we rewrite this as an equation for Γ^{pp}.

$$\Gamma^{pp}(p;p') = \Gamma(p;p'')$$

$$-(T/N\sum_{p''}\Gamma^{pp}(p;p'')G(p'')G(-p'')\Gamma(p'';p')$$

Once we have found the irreducible particle-particle Γ^{pp} and particle-hole Γ^{ph} vertices we can ask a variety of questions. Our primary focus will be on the structure of the pairing interaction

However, before doing this it is interesting to look at the leading eigenvalues of the Bethe-Salpeter equations in various channels.

The Bethe-Salpeter equation for the particle-particle channel with center of mass momentum Q=0 is

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

The Bethe-Salpeter equation for the particle-particle channel with center of mass momentum Q=0 is

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

In the same way, we have for the particle-hole channel with center of mass momentum Q

$$-(T/N)\sum_{p'}\Gamma^{ph}(p;p')G(p'+Q)G(p')\psi_\alpha(p') = \lambda_\alpha\psi(p)$$

with $\Gamma^{ph}(p;p')$ the irreducible particle-hole vertex .

At $\mathrm{T_c}$, the leading eigenvalue of the Bethe-Salpeter particle-particle channel goes to 1 and one has

$$\frac{\mathrm{T_c}}{\mathrm{N}}\sum_{\mathrm{k}'}\Gamma^{\mathrm{pp}}(\mathrm{k},\mathrm{k}')\,\mathrm{G}_\uparrow(\mathrm{k}')\,\mathrm{G}_\downarrow(-\mathrm{k}')\,\phi_{\mathrm{d}_{\mathrm{x}^2-\mathrm{y}^2}}(\mathrm{k}') = \phi_{\mathrm{d}_{\mathrm{x}^2-\mathrm{y}^2}}(\mathrm{k})\,.$$

Here, $k' = (k', \omega_{n'})$. This is the generalization of the usual BCS equation

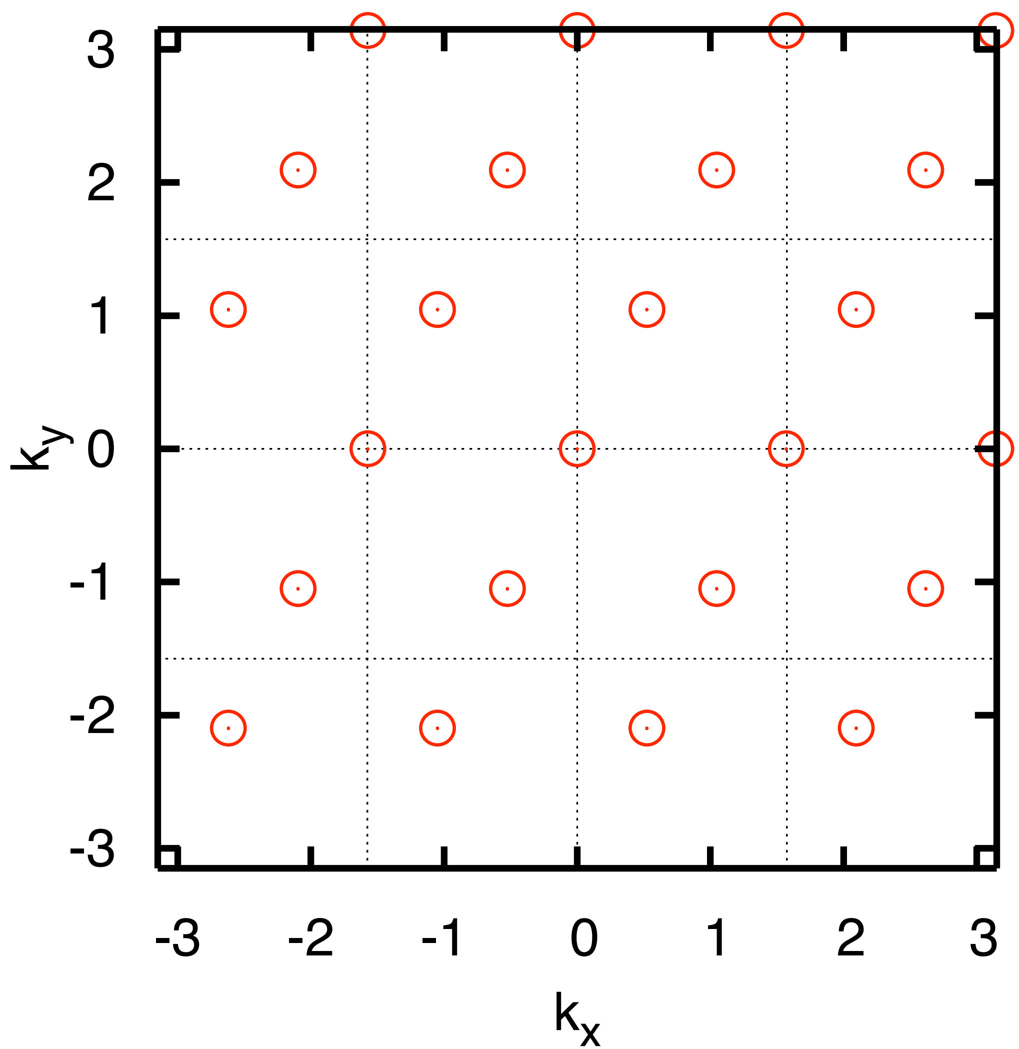
$$\frac{\mathrm{T_c}}{\mathrm{N}}\sum_{\mathrm{k}',\mathrm{n}'}\mathrm{V}_{\mathrm{kk}'}\frac{1}{\omega_{\mathrm{n}}^2+\varepsilon_{\mathrm{k}'}^2}\,\Delta_{\mathrm{k}'} = \Delta_{\mathrm{k}}$$

The following results were found for a Hubbard model with $U/t=4$ and $\langle n \rangle = .85$ using a dynamic cluster Monte Carlo approach developed by Mark Jarrell and his group at the University of Cincinnati.

M. Jarrell et al PRB 64 195130 (2001)

T. Maier et al cond-mat/0404055

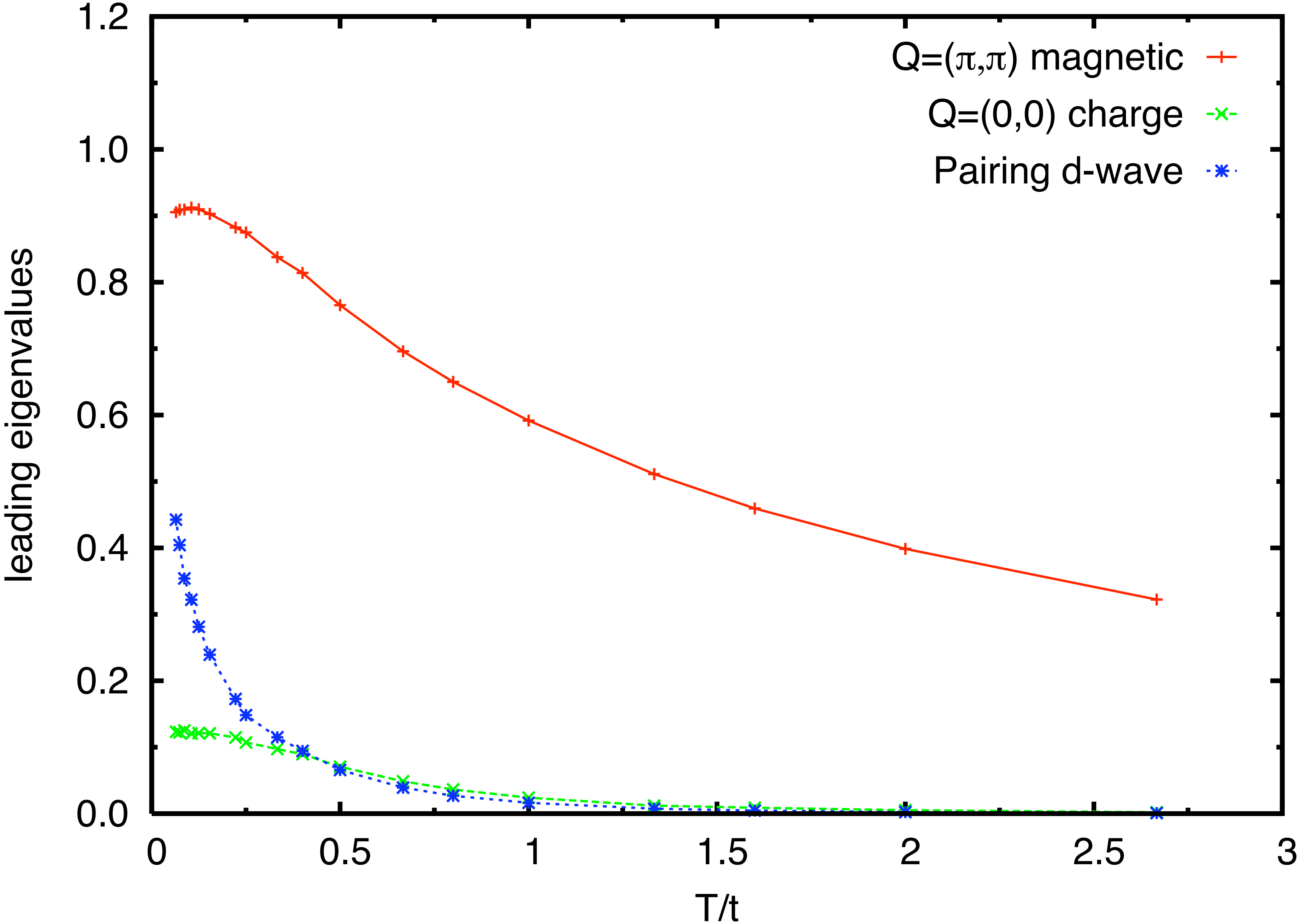
Cluster k-points



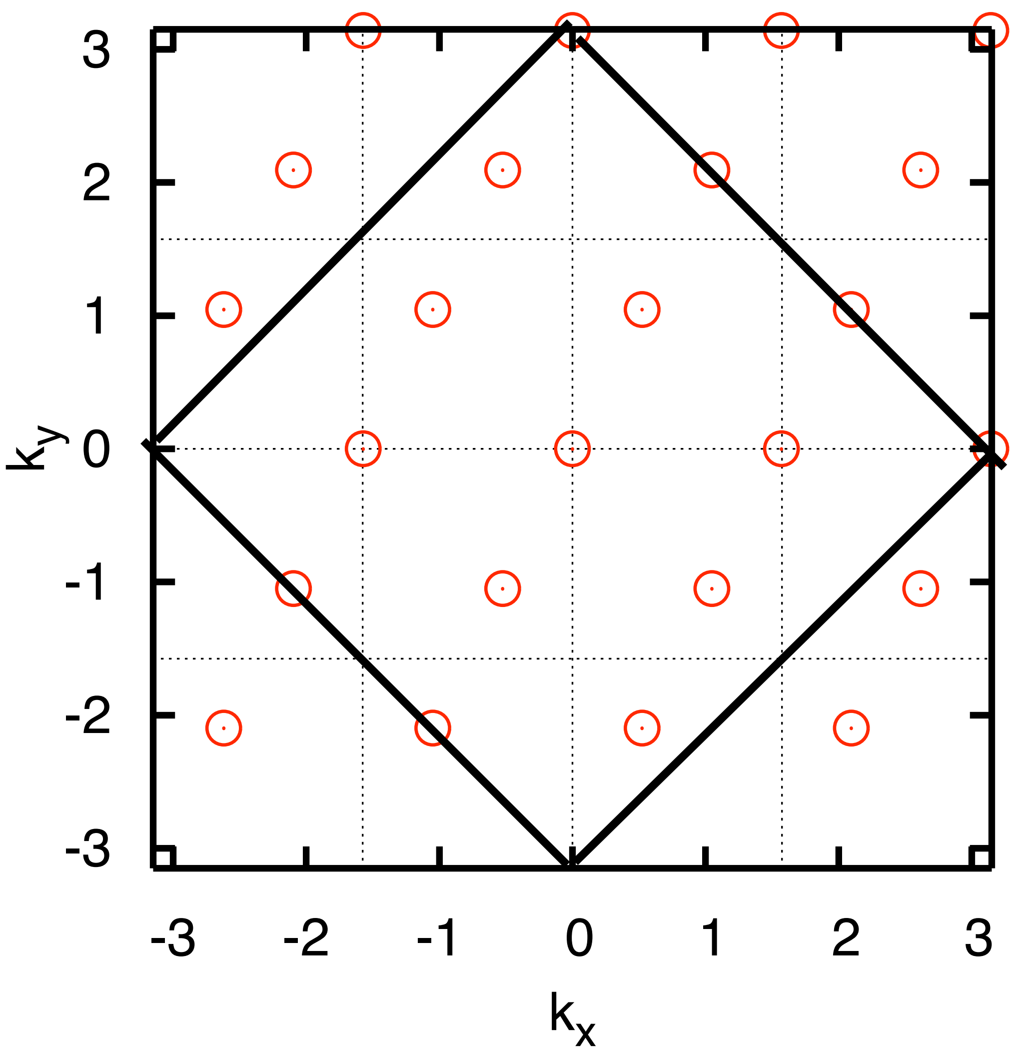
Can one understand the structure of the pairing interaction from the study of finite x or k-clusters at temperatures above Tc?

The pairing interaction is generally short range and retarded and becomes well developed at temperatures above Tc.

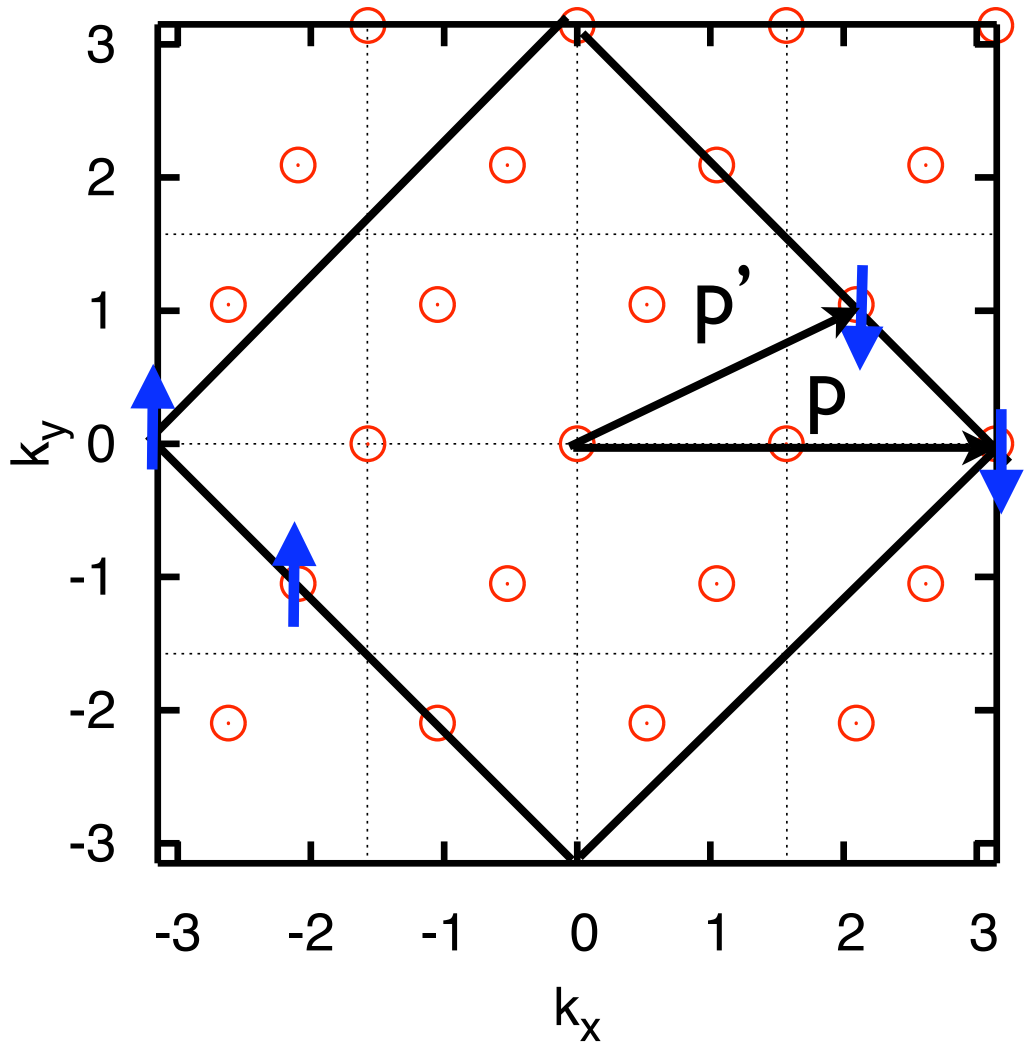
Leading Eigenvalues

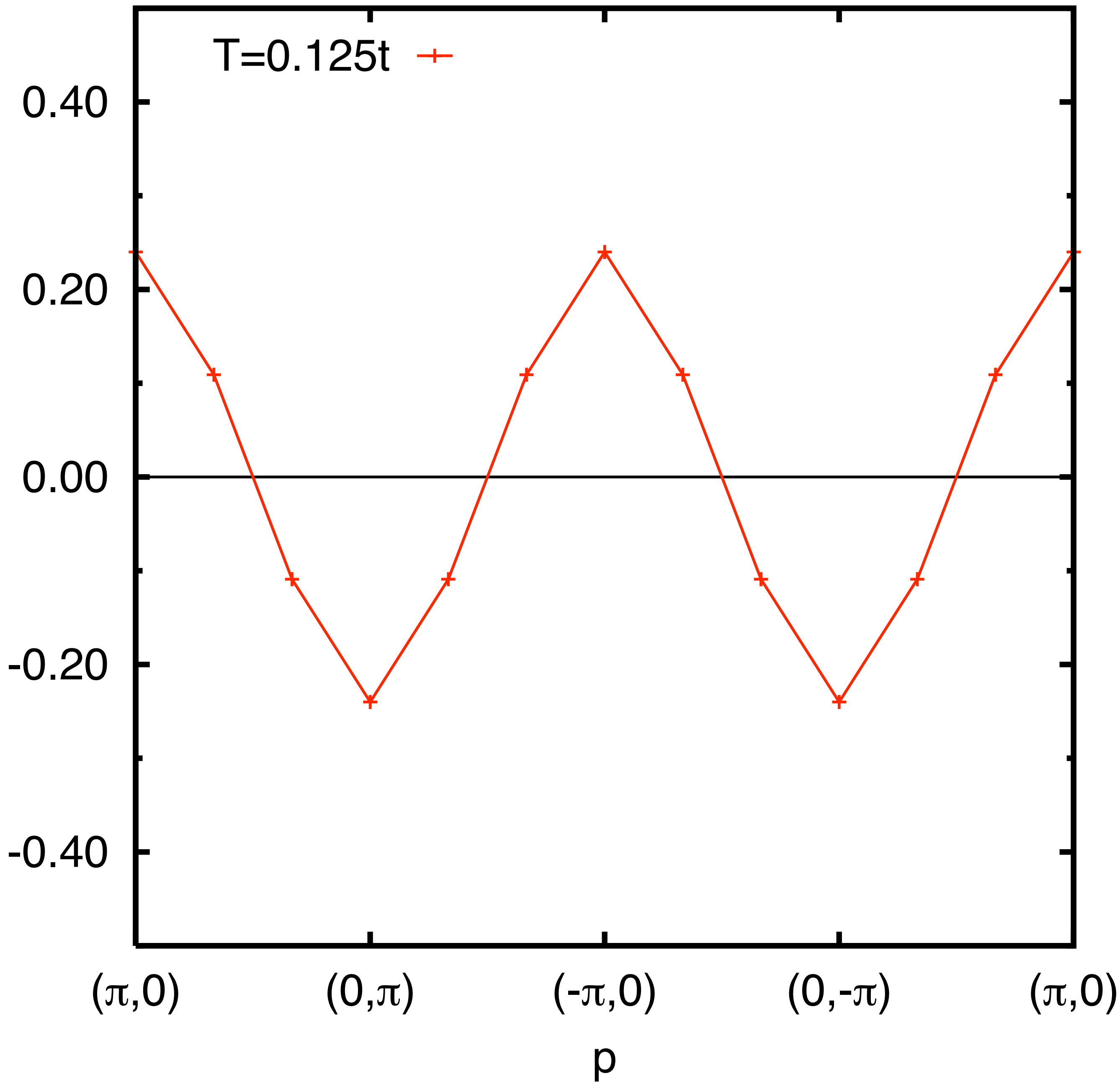


Cluster k-points

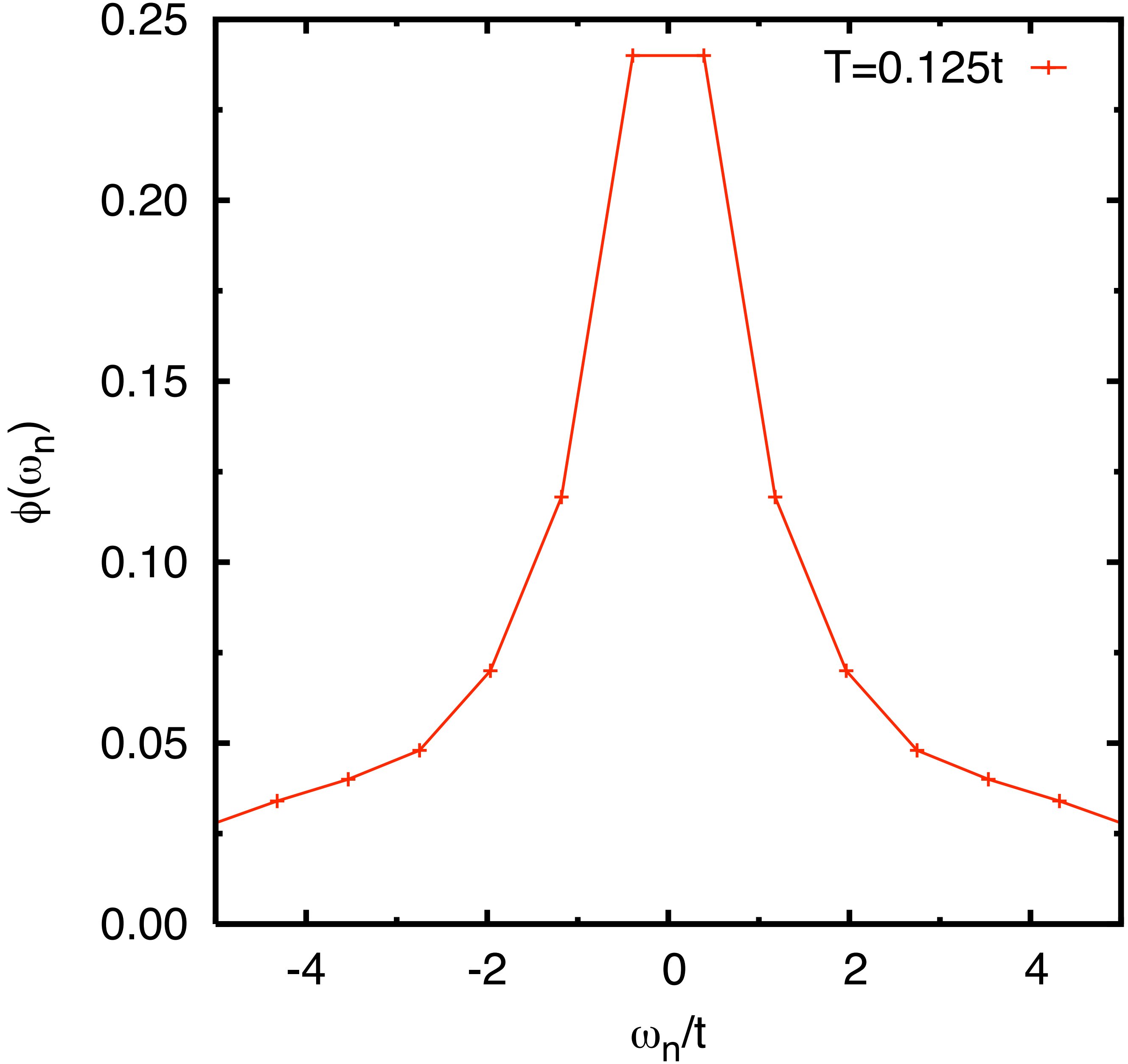


Cluster k-points





T=0.125t
0.40
0.20
0.00
-0.20
-0.40
φ(p,iπT)/t
(π,0)
(0,π)
(-π,0)
(0,-π)
(π,0)
p



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

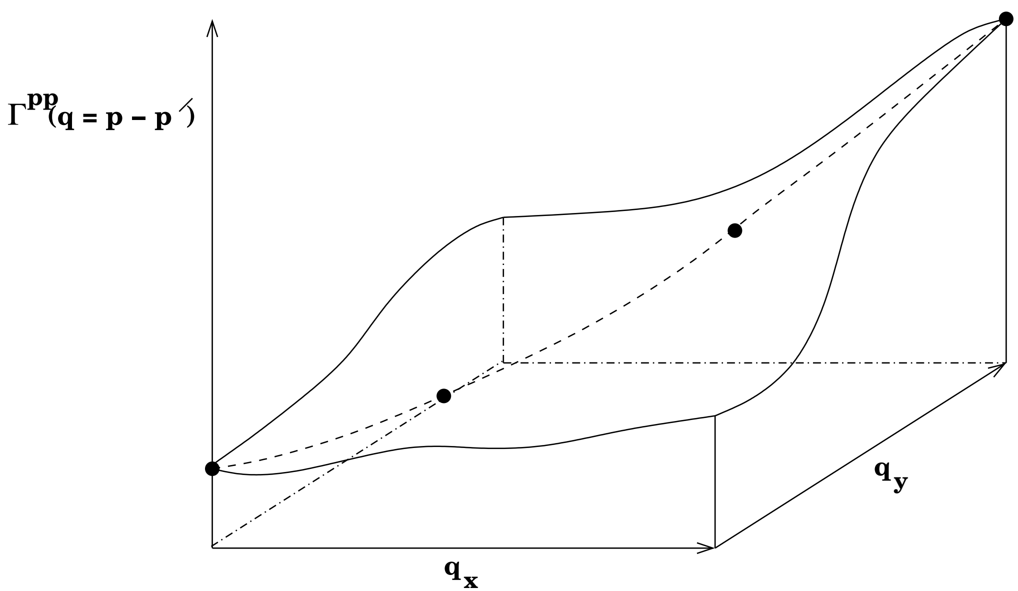
So the leading eigenvalue in the pairing channel has d(xx-yy) symmetry. What can one say about the interaction $\Gamma^{pp}(p;p')$ that causes this?

What is it’s momentum ,frequency and temperature dependence?

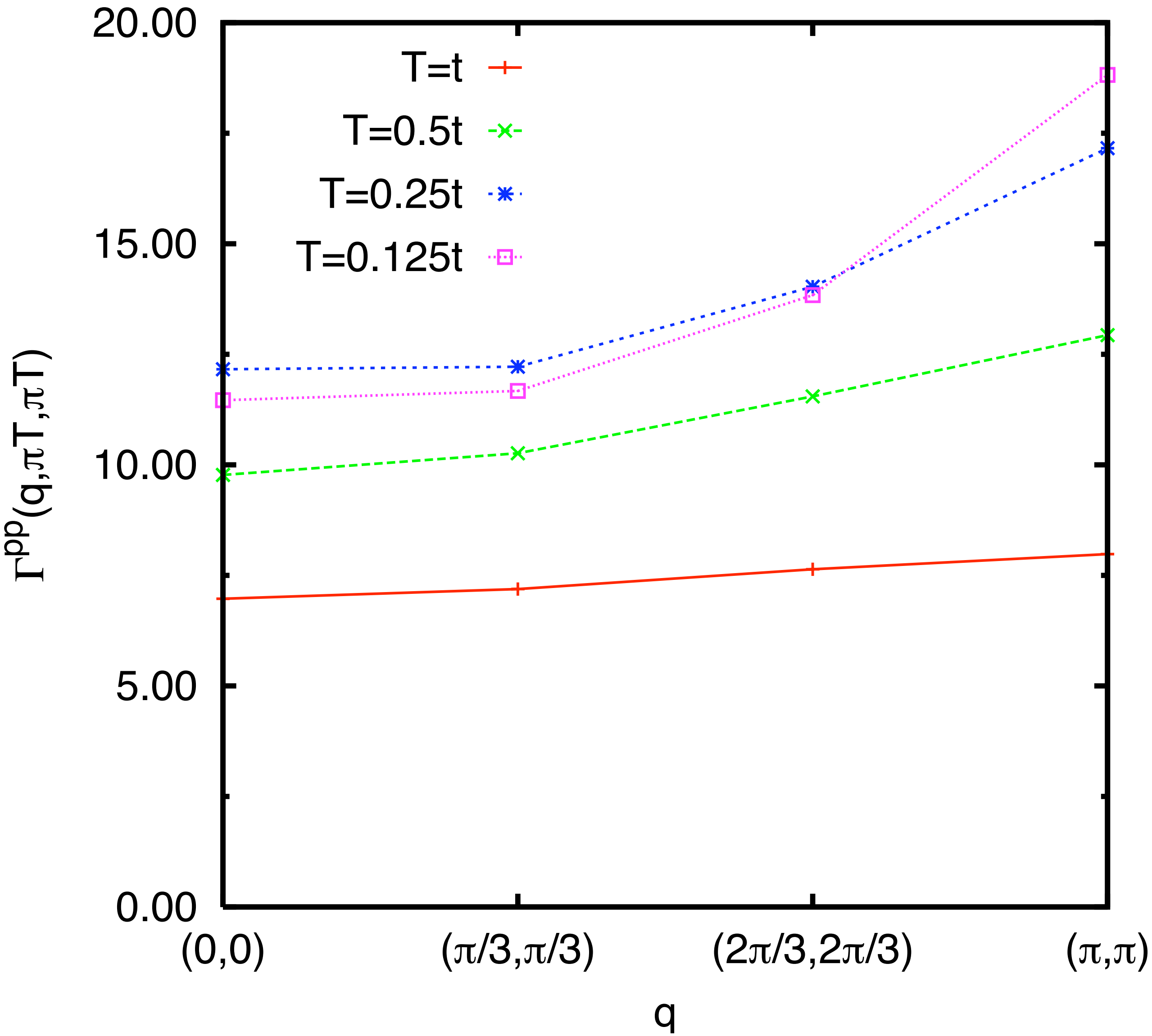
Is it associated with a particle-hole exchange channel? If so what is the spin of the channel?

Is it associated with an interaction that is not well described in such terms?

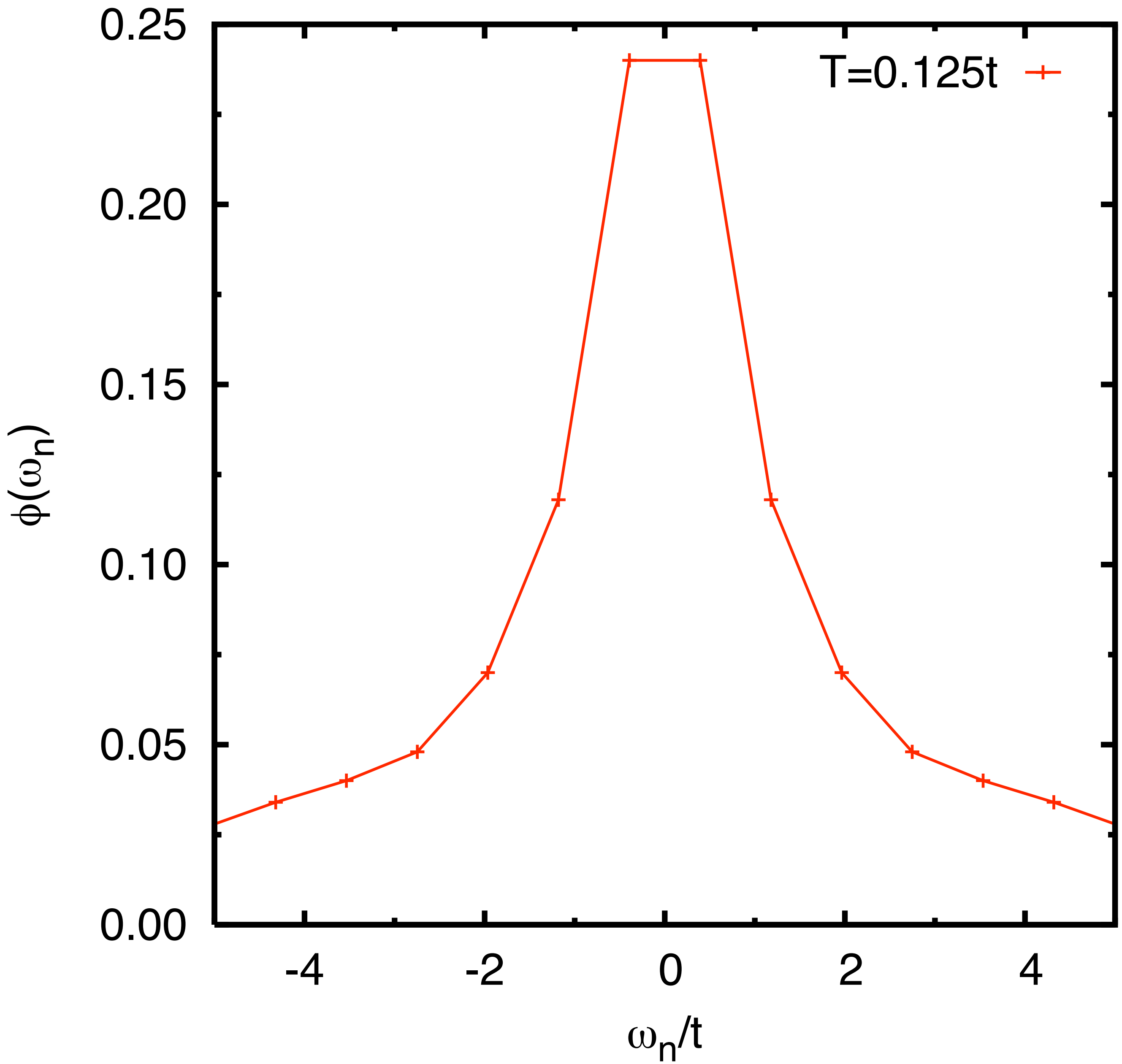
The momentum dependence of $\Gamma^{pp}(p;p')$ is shown schematically. The numerical data that I'll show is for points along qx=qy, with q=p-p'. The spatial Fourier transform of $\Gamma^{pp}(p;p')$ gives an interaction which is short range with the dominant terms being a repulsive onsite and an attractive near neighbor interaction.



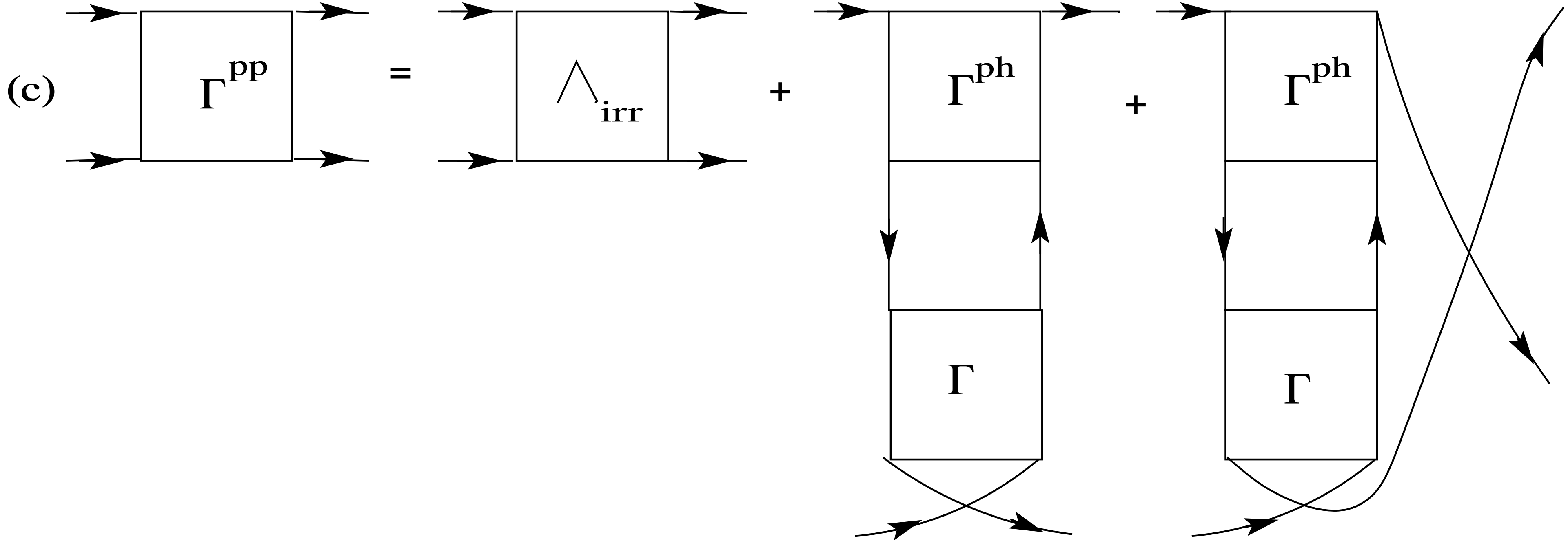
Momentum transfer dependence of $\Gamma^{pp}(p;p')$ for various temperatures



The frequency dependence of the irreducible particle-particle interaction is reflected in the ω_n dependence of the d(xx-yy) eigenfunction.



0.25
0.20
0.15
0.10
0.05
0.00
-4
-2
0
2
4
$\phi(\omega_n)$
ω_n/t
T=0.125t



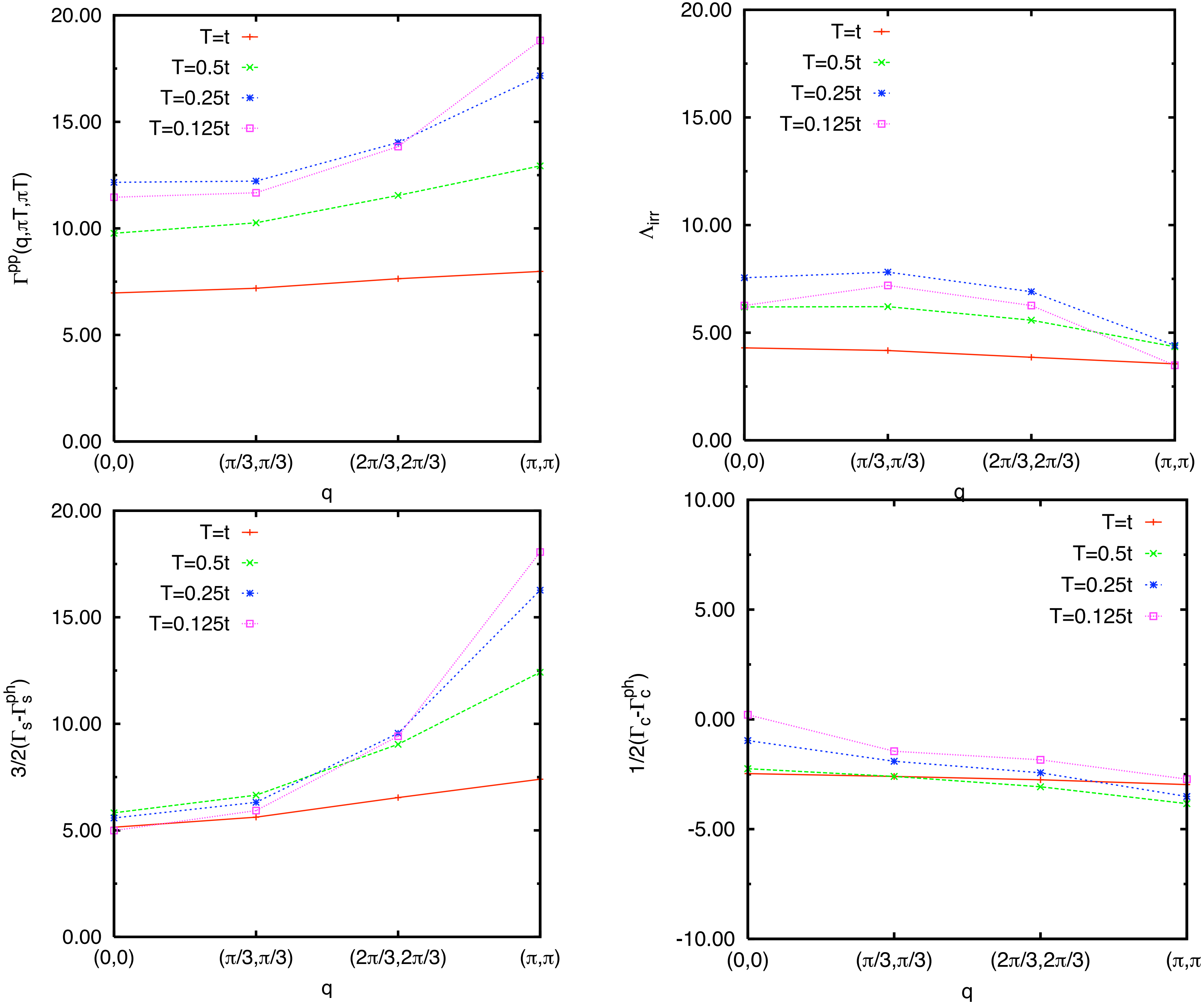
The irreducible particle-particle vertex can be decomposed into a "fully irreducible" vertex Λ_{irr},which is irreducible in all two-fermion channels and the sum of two particle-hole exchange contributions.

R. Haymaker and R. Blankenbecler, Phys Rev 171,1581 (1968)

G. Esirgen and N.E. Bickers,PRB 57, 5376

Because of the spin rotational invariance of the Hubbard model, the particle-hole channels can be separated into a charge density (S=0) and a magnetic spin (S=1) channel.

$$\Gamma^{pp}(p-p') = \Lambda_{irr}(p-p')$$
$$+(1/2)(\Gamma_c(p-p') - \Gamma_c^{ph}(p-p'))$$
$$+(3/2)(\Gamma_s(p-p') - \Gamma_s^{ph}(p-p'))$$



20.00
15.00
10.00
5.00
0.00
$\Gamma^{pp}(q,\pi T,\pi T)$
T=t
T=0.5t
T=0.25t
T=0.125t
(0,0)
(π/3,π/3)
(2π/3,2π/3)
(π,π)
q
20.00
15.00
10.00
5.00
0.00
Λ_{irr}
T=t
T=0.5t
T=0.25t
T=0.125t
(0,0)
(π/3,π/3)
(2π/3,2π/3)
(π,π)
q
20.00
15.00
10.00
5.00
0.00
$3/2(\Gamma_s-\Gamma_s^{ph})$
T=t
T=0.5t
T=0.25t
T=0.125t
(0,0)
(π/3,π/3)
(2π/3,2π/3)
(π,π)
q
10.00
5.00
0.00
-5.00
-10.00
$1/2(\Gamma_c-\Gamma_c^{ph})$
T=t
T=0.5t
T=0.25t
T=0.125t
(0,0)
(π/3,π/3)
(2π/3,2π/3)
(π,π
q

Conclusions

The effective pairing interaction in the 2D Hubbard model:

- leads to d(xx-yy) pairing
- increases with increasing momentum transfer (in real space it is repulsive for on site pairing and attractive for near neighbor singlet pairing)
- decreases when ω_m exceeds an effective exchange interaction energy (it is retarded on a time scale set by the inverse of an effective magnetic exchange energy)
- is mediated by a particle-hole spin S=1 channel

Some Questions

- Does a doped 2D Hubbard model actually have a superconducting phase and if this is the case, does it occurs at a "high" Tc ?
- Does one need an "enhancement" mechanism such as a striped nanostructure?
- Is there critical U beyond which the structure of the pairing interaction is qualitatively different?