Thermal conductivity of anisotropic spin ladders

By :Hamed Rezania

Razi University, Kermanshah, Iran

Magnetic Insulator

In one dimensional is a good candidate for thermal conductivity due to magnetic excitation

Partially filled electron shell : 3d,4d,4f,5f

Ferro: $CrBr_3$, K_2CuF_4, EuO, EuS, $CdCr_2Se_4$, Rb_2CrCl_4, etc.
Antiferro: $EuTe$, MnO, $RbMnF_3$, Rb_2MnCl_4, etc.
Ferri: $EuSe$, etc.

Heisenberg model Hamiltonian describes these material

$$H = J \sum_{\langle ij \rangle}' S_i S_j$$

Low dimensional quantum magnets

$$H_{Heisenberg} = J\sum_{i,j} S_i . S_j$$

1)Heisenberg chains
2) Spin ladders
3) Spin Peierls:

H=J$[1 + \delta(-1)^x]\mathbf{S}_x \cdot \mathbf{S}_{x+1}$

Spin liquid phase

1)Finite energy gap in magnetic excitation spectrum

2)Spatial Exponential behaviour for spin correlation function

$$\langle S_r . S_0 \rangle = e^{-r/\xi}$$

Sr2CuO3, SrCuO2

Electrically Insulating compounds Heisenberg chain

Thermal conductivity

Playground for magnetic studies of this material and quantum information processing and in electronic device

Transport of heat in insulator
1)Phonons
2) In low dimensions: magnetic excitation

$$K(\omega) = D\delta(\omega) + K_{reg}(\omega)$$

Integrable one dimensional

Ballistic Transport

Nonvanishing of Drude weight

Castella, etal: PRL 74, 972(1995)

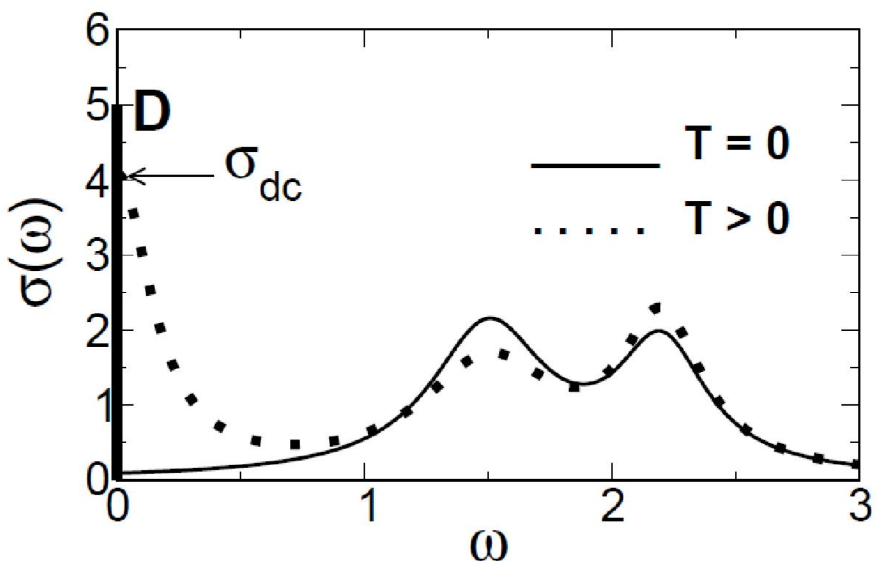
One dimensional quantum magnets show a unusually large thermal conductivity

$$(Sr, Ca, La)_{14}Cu_{24}O_{41}$$

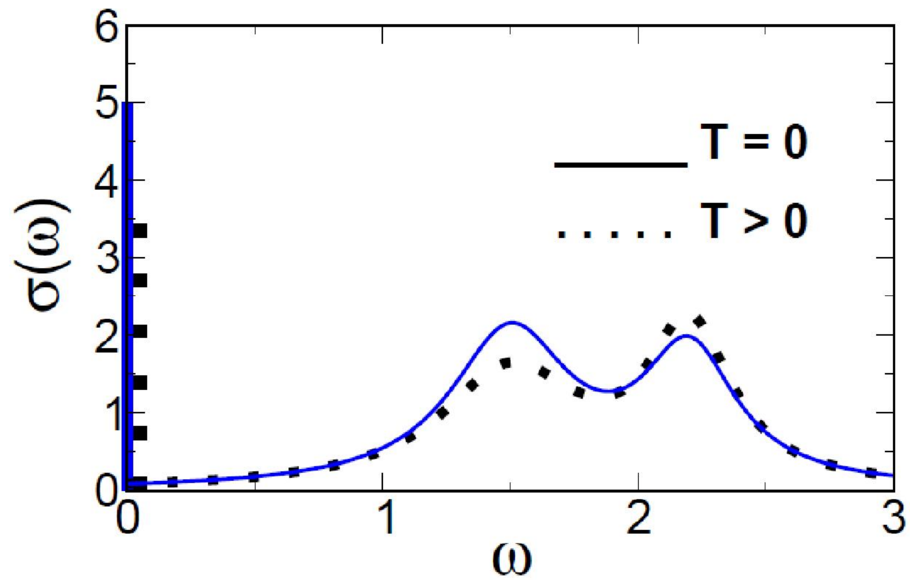
1D spin ladder

Nonitegrability with Luttinger fixed point
S. Fujimoto, PRL 90,19 (2003)

Ballistic and Diffusive Transport



Nonintegrable System



Integrable System

Nonzero Drude weight → Algebraic form for time correlation function between current functions

Zero Drude Weight → Exponential Behavior for time correlation function between

Three main cases at finite temperature:

$$(a) \qquad D_{11}(T) > 0; \quad \sigma_{\rm dc}(T) = 0$$
$$(b) \qquad D_{11}(T) > 0; \quad \sigma_{\rm dc}(T) > 0$$
$$(c) \qquad D_{11}(T) = 0; \quad \sigma_{\rm dc}(T) > 0\,.$$

Case (a) → Infinite Conductivity and exactly conserved current

Case (b) → $j_1 = j_c + j_{\rm dec}\,,$

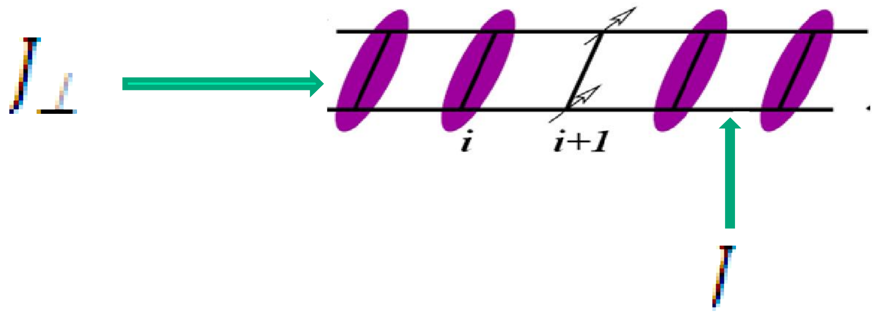
Case (c) → Exponential decay for current-current correlation function with full dissipation for current

Anisotropic spin ladder model Hamiltonian

Because of crystal field effects and easy axis effect, we introduce two global and local anisotropies: δ, Δ

$$\mathcal{H} = J_{\perp} \sum_i (S_i^x \tau_i^x + S_i^y \tau_i^y + \Delta S_i^z \tau_i^z) + J \sum_i (\tau_i^x \tau_{i+\delta}^x + \tau_i^y \tau_{i+\delta}^y + \delta \tau_i^z \tau_{i+\delta}^z)$$

$$+ J \sum (S_i^x S_{i+\delta}^x + S_i^y S_{i+\delta}^y + \delta S_i^z S_{i+\delta}^z).$$



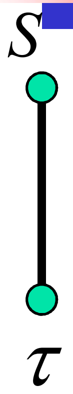
τ S are the spin operator of localized electrons on each chain

and the coupling constants $J, J_{\perp}$ are

antiferromagnetic type.

Bond operator Representation

S. Sachdev and R. Bhatt, PRB 41, 9332(1990)



$$s^{+}|0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$t_x^{+}|0\rangle = -\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)$$

$$t_y^{+}|0\rangle = \frac{i}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$$

$$t_z^{+}|0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$S^{\alpha} = \frac{1}{2}(s^{\dagger}t_{\alpha} + t_{\alpha}^{\dagger}s - i\,\varepsilon_{\alpha\beta\gamma}t_{\beta}^{\dagger}t_{\gamma})$$

$$\tau^{\alpha} = \frac{1}{2}(-s^{\dagger}t_{\alpha} - t_{\alpha}^{\dagger}s - i\,\varepsilon_{\alpha\beta\gamma}t_{\beta}^{\dagger}t_{\gamma})$$

$$[S_{\alpha}, S_{\beta}] = i\varepsilon_{\alpha\beta\gamma}S_{\gamma}$$

$$s^{\dagger}s + t_{\alpha}^{\dagger}t_{\alpha} = 1$$

$$\left[t_{\alpha}, t_{\beta}^{\dagger}\right] = \delta_{\alpha\beta}$$

Constraint

Bosonic Representation

The parts of hamiltonian after applying Bond operator transformation

$$\mathcal{H}_{bil} = \sum_{\mathbf{k},\alpha=\mathbf{x},\mathbf{y},\mathbf{z}} A_{\mathbf{k},\alpha} t^{\dagger}_{\mathbf{k},\alpha} t_{\mathbf{k},\alpha} + \sum_{\mathbf{k},\alpha=\mathbf{x},\mathbf{y},\mathbf{z}} \frac{B_{\mathbf{k},\alpha}}{2} (t^{\dagger}_{\mathbf{k},\alpha} t^{\dagger}_{-\mathbf{k},\alpha} + h.c.)$$

With coefficients:

$$\begin{aligned} A_{\mathbf{k},(\mathbf{x},\mathbf{y})} &= J_{\perp}(\frac{1+\Delta}{2}) + Jcos(k_x), \quad A_{\mathbf{k},\mathbf{z}} = J_{\perp} + \delta J cos(k_x) \\ B_{\mathbf{k}} &= -Jcos(k_x), \quad B_{\mathbf{k},\mathbf{z}} = J\delta cos(k_x). \end{aligned}$$

Green's function formalism

Interacting one particle Green's function :

$$\Omega_{k,\alpha} = Z_{k,\alpha}\sqrt{(A_{k,\alpha} + \Sigma_{n,\alpha}(k,0))^2 - (B_{k,\alpha} + \Sigma_{a,\alpha}(k,0))^2}$$

$$G_\alpha(k,\omega) = \frac{Z_{k,\alpha}U^2_{k,\alpha}}{\omega - \Omega_{k,\alpha} + i\delta} - \frac{Z_{k,\alpha}V^2_{k,\alpha}}{\omega + \Omega_{k,\alpha} - i\delta}$$

$\Sigma_{n,\alpha}(k,0), \Sigma_{a,\alpha}(k,0)$ is normal and anomalous self energies and $Z_{k,\alpha}$ is renormalization constant.

$$Z^{-1}_{k,\alpha} = 1 - \frac{\partial \Sigma_{n,\alpha}(k,0)}{\partial \omega}$$

Interacting Bogoliubov coefficients:

$$U^2_{k,\alpha}, V^2_{k,\alpha} = +,-\frac{1}{2} + \frac{A_{k,\alpha} + \Sigma_{n,\alpha}(k,0)}{2\Omega_{k,\alpha}}$$

Finite temperature Calculations

Dilution of triplet gas $\rightarrow$ $T \ll J, J_{\perp}$

Matsubara's Green's functions

$$g_{n,\alpha}(k,\tau) = -\langle T_{\tau}[t_{k,\alpha}(\tau)t^{\dagger}_{k,\alpha}(0)]\rangle$$

$$g_{a,\alpha}(k,\tau) = -\langle T(t^{\dagger}_{k,\alpha}(\tau)t^{\dagger}_{-k,\alpha}(0))\rangle$$

$$G^{\mathrm{Ret}}_{\alpha}(k,\omega) = g_{\alpha}(k, i\omega_n \rightarrow \omega + i\delta) = \frac{Z_{k,\alpha}U^2_{k,\alpha}}{\omega - \Omega_{k,\alpha} + i\eta} - \frac{Z_{k,\alpha}V^2_{k,\alpha}}{\omega + \Omega_{k,\alpha} + i\eta}$$

Interacting one particle Green's function :

$$\Omega_{k,\alpha} = Z_{k,\alpha}\sqrt{\{A_{k,\alpha} + \mathrm{Re}[\Sigma^{\mathrm{Ret}}_{n,\alpha}(k,0)]\}^2 - \{B_{k,\alpha} + \mathrm{Re}[\Sigma^{\mathrm{Ret}}_{a,\alpha}(k,0)]\}^2}$$

renormalization constant: $$Z^{-1}_{k,\alpha} = 1 - \left(\frac{\partial\, \mathrm{Re}(\Sigma^{\mathrm{Ret}}_{n,\alpha})}{\partial \omega}\right)_{\omega=0}$$

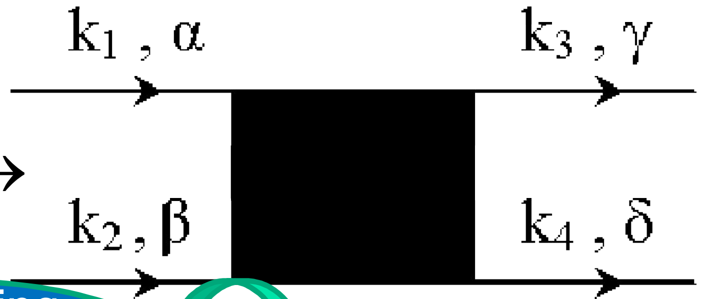
Interacting Bogoliubov coefficients: $$U^2_{k,\alpha}(V^2_{k,\alpha}) = (-)\frac{1}{2} + \frac{Z_{k,\alpha}\{A_{k,\alpha} + \mathrm{Re}[\Sigma^{\mathrm{Ret}}_{n,\alpha}(k,0)]\}}{2\Omega_{k,\alpha}}$$

Calculation of hard core self-energy

Brueckner approach [Fetter & Walecka] for finding self energy of dilute Boson gas in the hard core condition :

$$H_U = U \sum_{i,\alpha,\beta} t^{\dagger}_{\alpha i} t^{\dagger}_{\beta i} t_{\beta i} t_{\alpha i}, \qquad U \to \infty$$

$$\Gamma^{\alpha\beta,\gamma\delta}(K = k_1 + k_2) \to$$



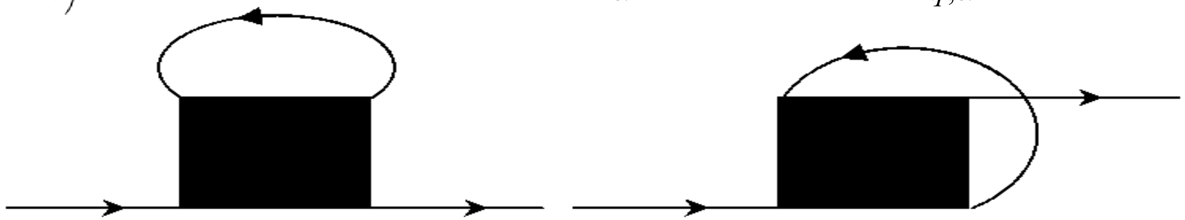
Vertex function (Scattering amplitude)

Neglecting anomalous GF

$$\sum_{\alpha} \left\langle t^{+}_{\alpha,i} t_{\alpha,i} \right\rangle = \frac{1}{N} \sum_{q,\alpha} v^2_{q,\alpha} \approx 0.1$$

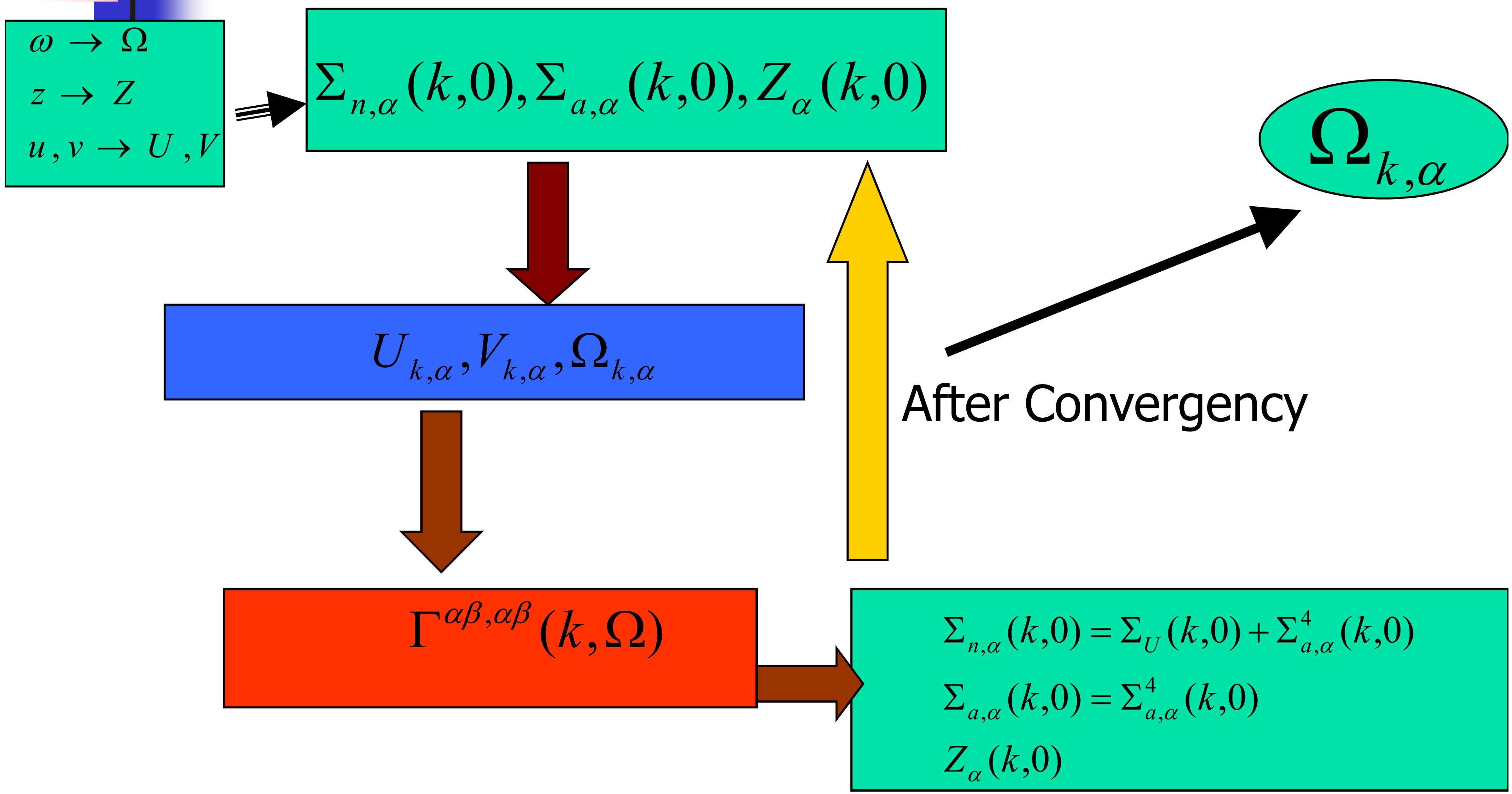
$$\Gamma_{\alpha\beta,\alpha\beta}(\mathbf{K}, i\omega_n) = \left(\frac{1}{\beta 2\pi} \sum_{Q_m} \int d^3Q G^{(0)}_{\alpha\alpha}(Q) G^{(0)}_{\beta\beta}(K-Q) \right)^{-1}$$

Hard core part of self energy:



$$\Sigma^U_{\alpha\alpha}(\mathbf{k}, i\omega_n) = -\sum_{p_m,\gamma} \int_{-\infty}^{\infty} \frac{dp}{2\pi\beta} \Gamma(p,k;p,k)_{\alpha\gamma,\alpha\gamma} G_{\gamma\gamma}(p) - \sum_{p_m} \int_{-\infty}^{\infty} \frac{dp}{2\pi\beta} \Gamma(p,k;k,p)_{\alpha\alpha,\alpha\alpha} G_{\alpha\alpha}(p)$$

Self-Consistent loop



Energy current and thermal conductance

Energy current is obtained based on the following definition

$$\mathbf{R}_E \equiv \sum_i \mathbf{R}_i h_i,$$

h_i Local hamiltonian

$\mathbf{R}_i$ denotes the position of a rung on the lattice

$$H = \sum_m h_m,$$

$$h_m = J(S^x_m S^x_{m+a} + S^y_m S^y_{m+a} + \delta S^z_m S^z_{m+a} + \tau^x_m \tau^x_{m+a} + \tau^y_m \tau^y_{m+a} + \delta \tau^z_m \tau^z_{m+a}) + J_\perp (S^x_m \tau^x_m + S^y_m \tau^y_m + \Delta S^z_m \tau^z_m)$$

Energy conservation equation

$$\mathbf{J}_E = \frac{\partial}{\partial t}\mathbf{R}_E = \sum_l \mathbf{R}_l \frac{\partial}{\partial t} h_l = i \sum_{l,m} \mathbf{R}_l [h_m, h_l]$$

Kubo Formula for thermal conductivity

$$J_{Q,\alpha} = -\frac{1}{T} L^{21}_{\alpha\delta} \nabla_\delta (eV) + L^{22}_{\alpha\delta} \nabla_\delta \frac{1}{T}$$

$$L^{Ret}_{22}(\omega) = \frac{i}{\beta\omega} \int_{-\infty}^{+\infty} dt e^{i\omega t} \theta(t) \langle [j^x_E(t), j^x_E(0)] \rangle = \frac{1}{\beta\omega} \lim_{i\omega_n \longrightarrow \omega + i0^+} \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau (j^x_E(\tau) j^x_E(0)) \rangle$$

Thermal conductivity $\Longrightarrow$ $K = -\beta^2 \lim_{\omega \longrightarrow 0} Im(L^{Ret}_{22}(\omega))$

$$\kappa(i\omega_n) = \frac{-12J^4}{L^2\beta^2} \sum_{k,k',n_1,n_2} \zeta(k_x, k'_x) \chi^{xx}(k, i\omega_{n_1}) \chi^{yy}(k', i\omega_{n_2}) \chi^{zz}(k' + k, i\omega_n - i\omega_{n_1} - i\omega_{n_2})$$

$$\zeta(k_x, k'_x) \equiv 1 + \delta e^{-3ik_x} + \delta^2 e^{-3i(k_x + k'_x)} - \delta^2 e^{i(k'_x - k_x)} - \delta e^{-i(k_x + 2k'_x)} - \delta^2 e^{-2i(k'_x + 2k_x)},$$

Spin susceptibility

$$\chi_{zz}(k,i\omega_n) = -\int_0^\beta d\tau e^{i\omega_n\tau}\langle T(S_z(k,\tau)S_z(-k,0))\rangle$$

$$= \frac{1}{4}\int_0^\beta d\tau e^{i\omega_n\tau}$$

$$\Big\langle T\Big(t_{-k,z}(\tau)+t^\dagger_{k,z}(\tau)+\sum_q(-it^\dagger_{k+q,x}(\tau)t_{q,y}(\tau)+it^\dagger_{k+q,y}(\tau)t_{q,x}(\tau))\Big)\times$$

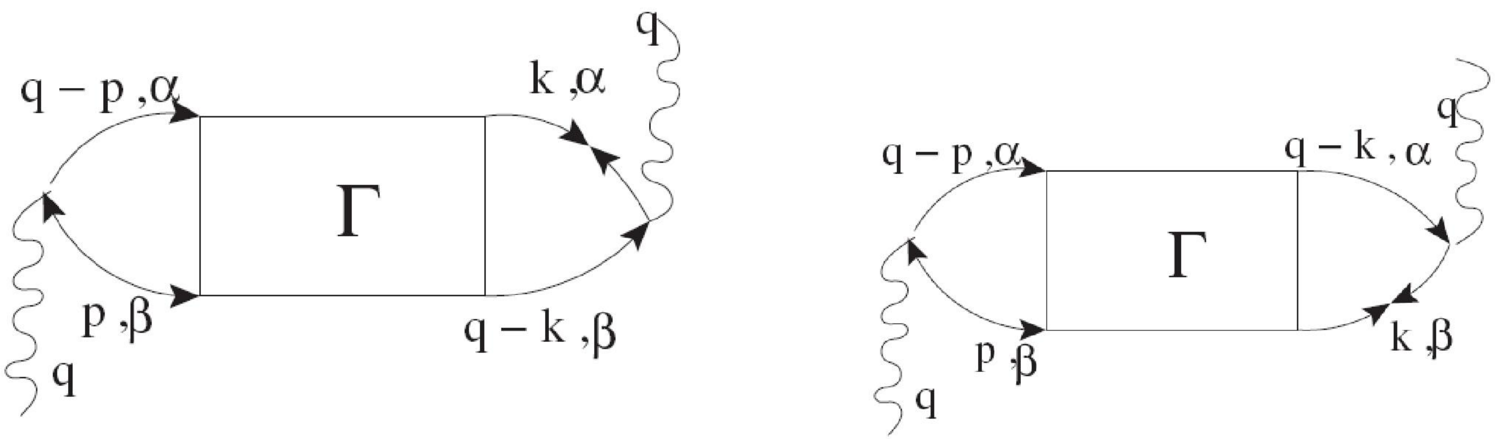
$$\Big(t_{k,z}(0)+t^\dagger_{-k,z}(0)+\sum_{q'}(-it^\dagger_{k-q',x}(0)t_{q',y}(0)+it^\dagger_{q'-k,y}(0)t_{q',x}(0))\Big)\Big\rangle.$$

1)One particle bosonic Green's function
2)Two particle bosonic Green's function

$$\chi_{zz}(k,i\omega_n) = \frac{1}{4}\Big(u^2_{k,z}(\frac{1}{i\omega_n-\omega_{k,z}}-\frac{1}{i\omega_n+\omega_{k,z}})-2u^2_{q,x}u^2_{k+q,x}\frac{n_B(\omega_{q,x})-n_B(\omega_{k+q,x})}{i\omega_n-\omega_{k+q,x}+\omega_{q,x}}\Big).$$

Vertex correction

Neglecting the below diagrams due to anomalous Green's function in the diagrams structures

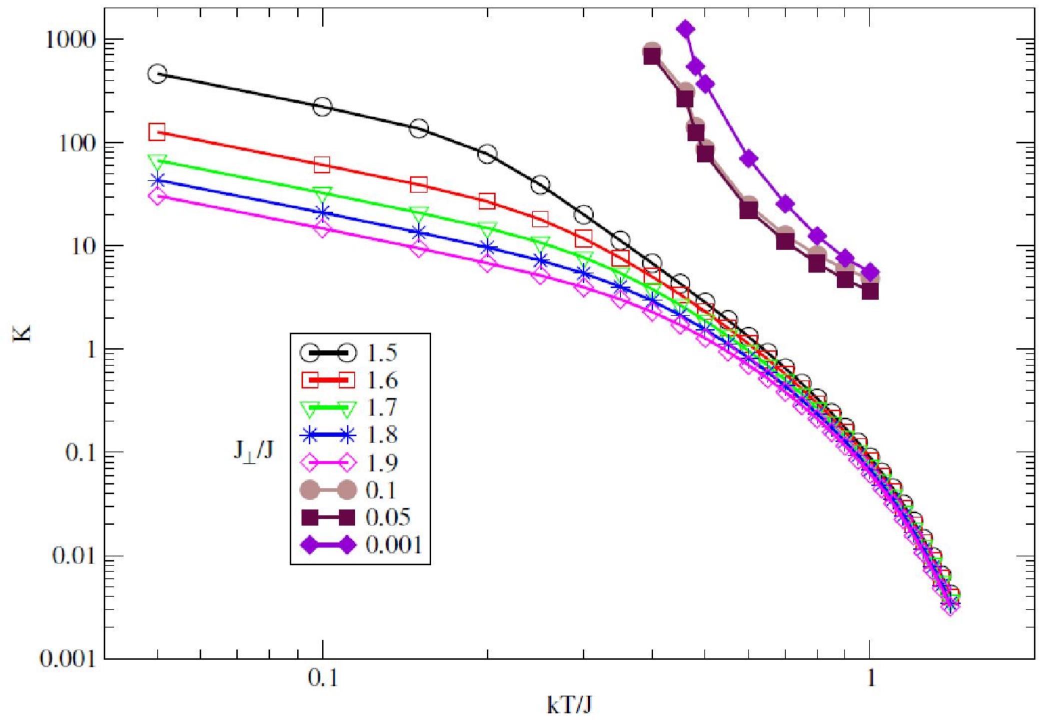


Numerical Results

After solving the equations self consistently → Obtaining the Interacting green's function and thermal conductance

Thermal conductivity of isotropic case versus temperature for various coupling constants.

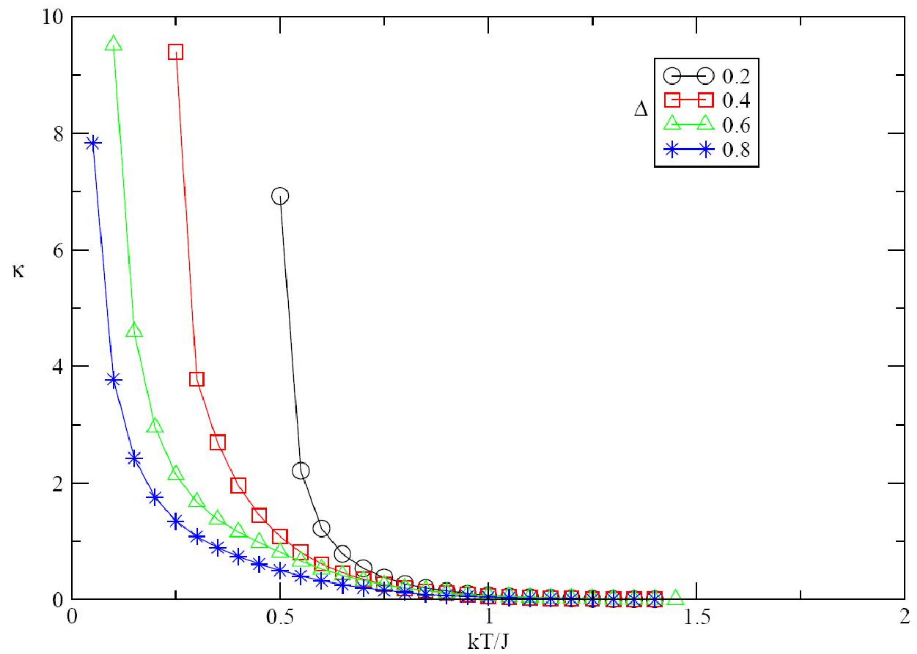
Monotonic decreasing with temperature



Decreasing conductance with $J_\perp$

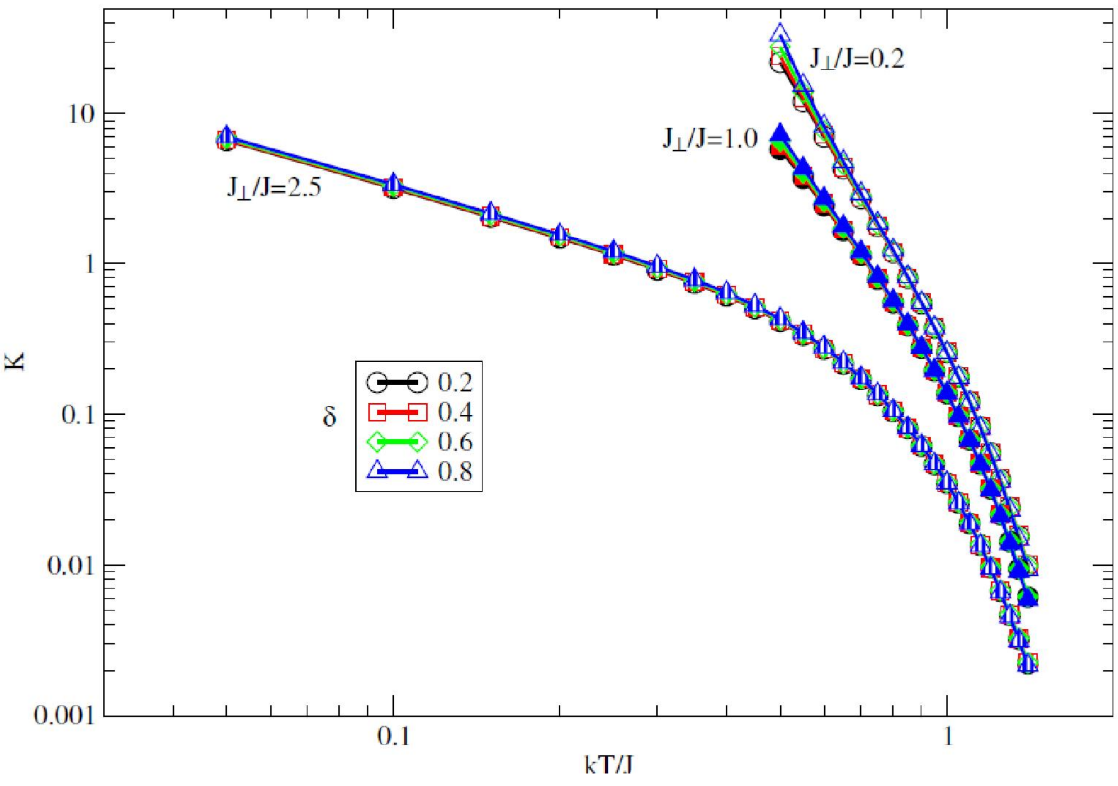
The effect of local anisotropy

Noticeable change of conductivity with local anisotropy



The effect of global anisotropy

There is no considerable change due to inter chain anisotropy



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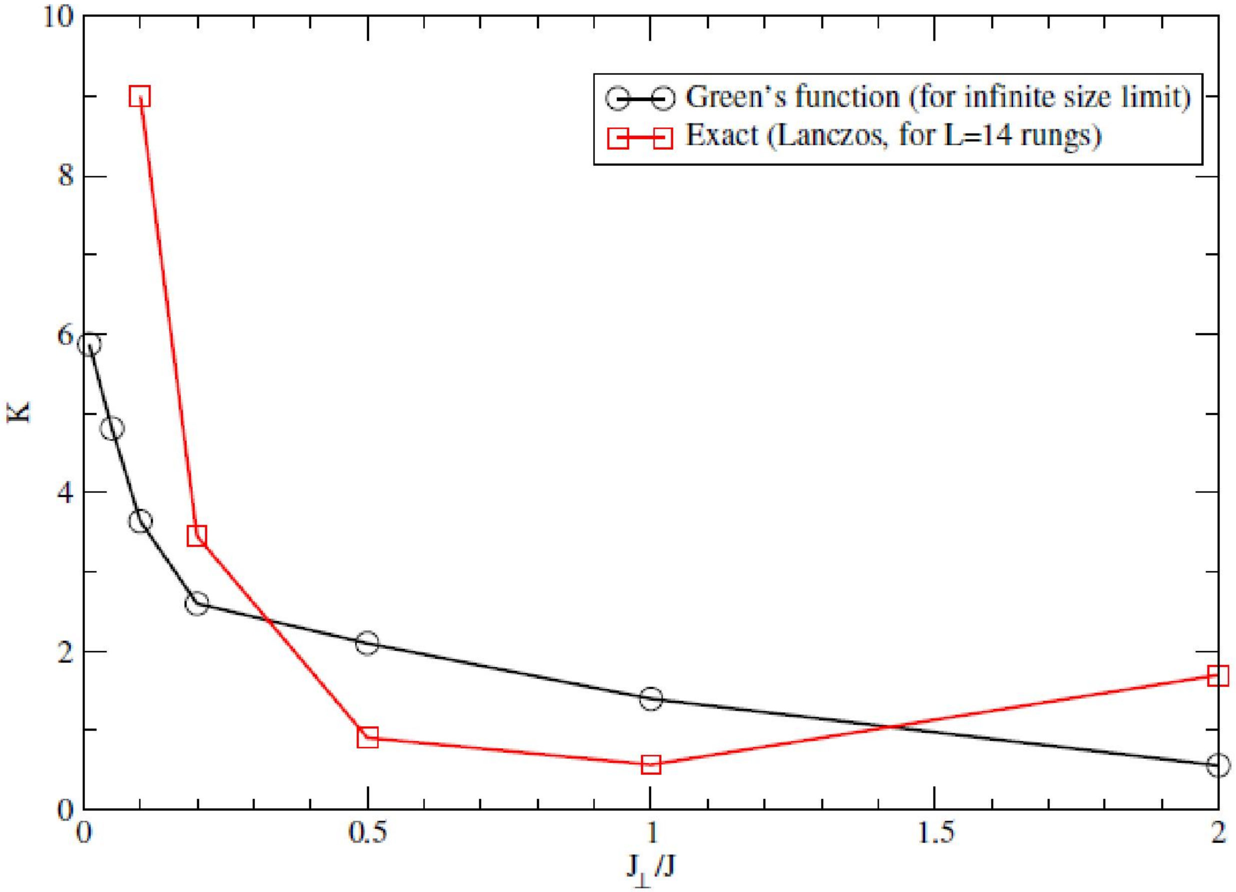

Green's function (for infinite size limit)
Exact (Lanczos, for L=14 rungs)
K
J⊥/J
0
2
4
6
8
10
0
0.5
1
1.5
2