A method for Computation of Thermal Conductivty

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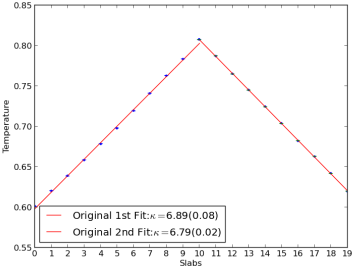
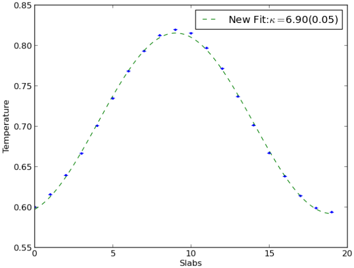
Overview

Introduction





Theory

$$J_x(x) = \frac{1}{\Omega} \sum_Q \hbar\omega v_{Qx} N_Q(x)$$

$$J_x(q) = -\kappa(q) \nabla T(q)$$

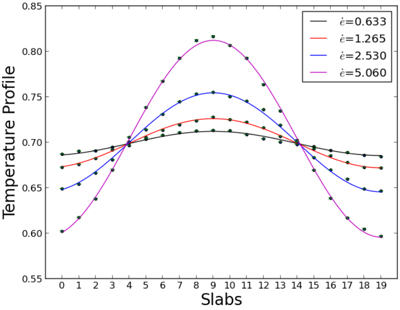
$$\Longrightarrow$$

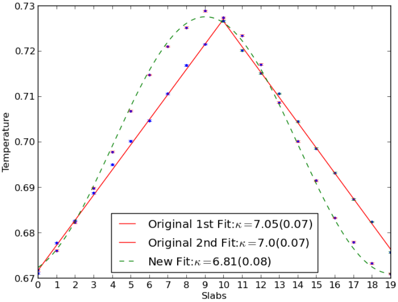
$$\kappa(q) = \frac{1}{\Omega} \sum_Q \frac{\hbar\omega v_{Qx}^2 (\partial n_Q / \partial T)}{1/\tau_Q + iqv_{Qx}} \nabla T(q) \longrightarrow q \to 0$$

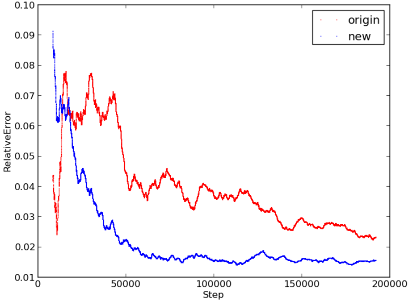
$$\Longrightarrow$$

$$\kappa(x - x') = \frac{1}{\Omega} \sum_Q^{v_{Qx}>0} \hbar\omega_{Qx} v_{Qx} e^{-|x-x'|/v_{Qx}\tau_Q}$$

Test on Liquid



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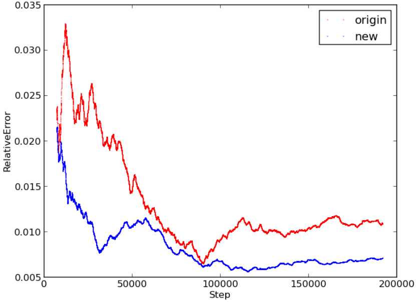
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
RelativeError
0
50000
100000
150000
200000
Step
origin
new


0.035
0.030
0.025
0.020
0.015
0.010
0.005
RelativeError
0
50000
100000
150000
200000
Step
origin
new

Theory:Debye Model

$\kappa(q)$

$$\kappa(q) = \frac{1}{\Omega}\sum_{Q}\hbar\omega\frac{\partial n_Q}{\partial T}v_{Qx}^2\tau_Q \times [\frac{1}{1+(qv_{Qx}\tau_Q)^2}]$$

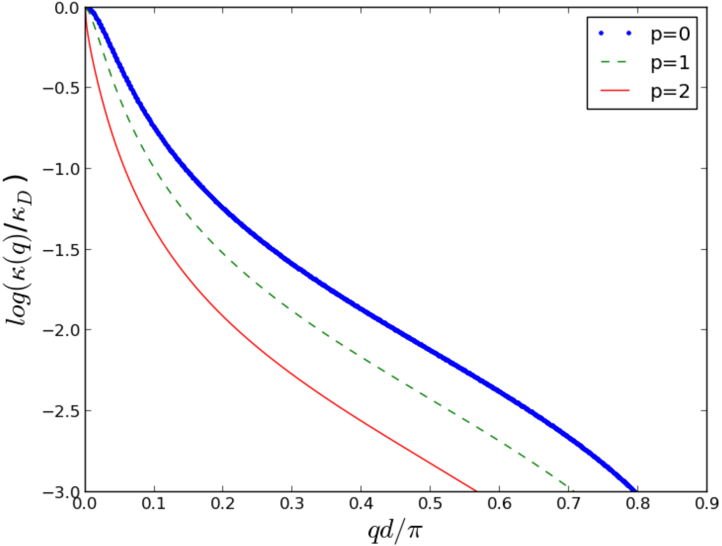
$$|v_Q| = v$$

$$\tau_Q, \Lambda_Q \propto \left(\frac{\omega_D}{\omega}\right)^p, p = 0, 1, 2, 3, 4$$

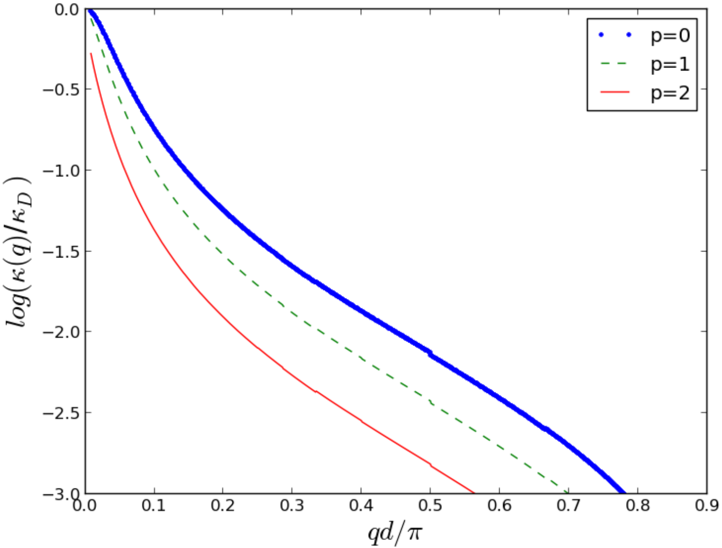
κ_D:Thermal Conduction in Debye Model

$$\kappa = \frac{1}{3}v\int_0^{\omega_D}\Lambda(\omega)c\omega d\omega = \frac{3}{3-p}\times\Lambda_{min}\times C_\infty$$

Infinite Crystal



Finite Model



Finite Model

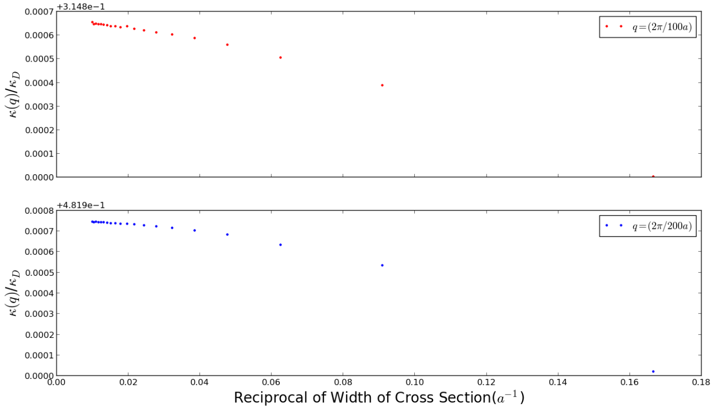
$$\kappa(q) = \frac{1}{\Omega}\sum_{Q}\hbar\omega\frac{\partial n_Q}{\partial T}v_{Qx}^2\tau_Q \times [\frac{1}{1+(qv_{Qx}\tau_Q)^2}]$$

Summing up in the 1st Brillouin Zone

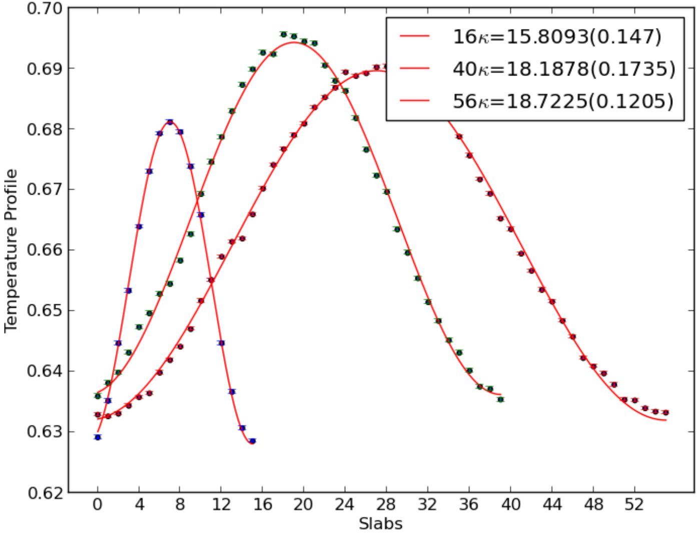
$$\longrightarrow$$

$$kappa(q) \to \kappa_D$$

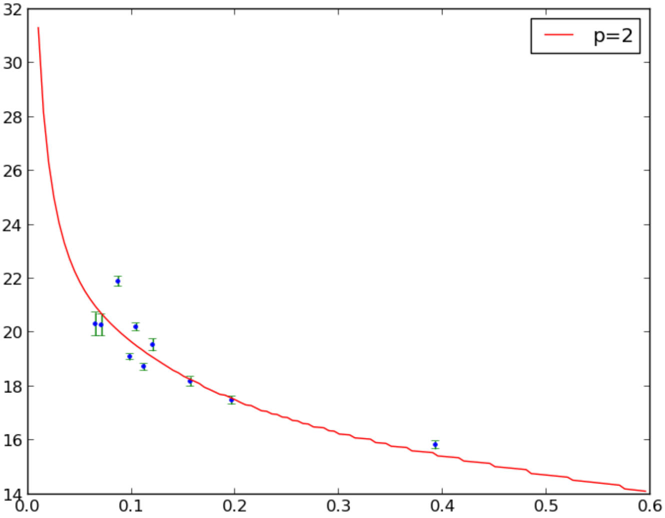
Cross Section



Test on Crystal



Test on Crystal



Conclusion

Conclusion 1

The sine temperature profile converges faster than the simple input at two ends.

Conclusion 2

The treatment of solution from PBE does not need very large cross section.

Conclusion 3

This method of extrapolation is expected to give a reasonable result.

The End