# Heat Transport in Nanoscales

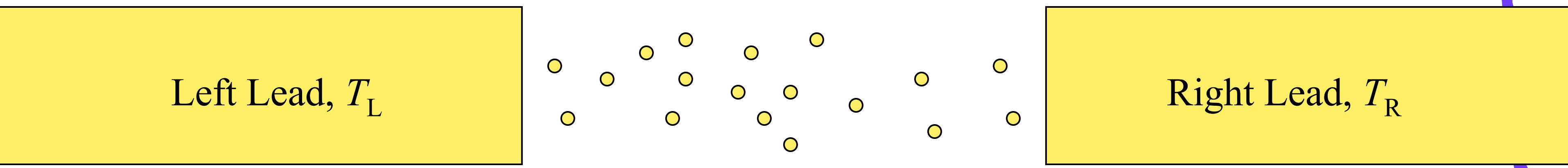
**Jian-Sheng Wang**

National University of Singapore, Institute of High Performance Computing, and Singapore-MIT Alliance

# Outline

- Brief review of theories and computational methods for thermal transport
- Report of some of our recent results (MD, ballistic/diffusive transport in nano-tubes)
- Nonequilibrium Green's function method
- Conclusion

# Thermal Conduction at a Junction



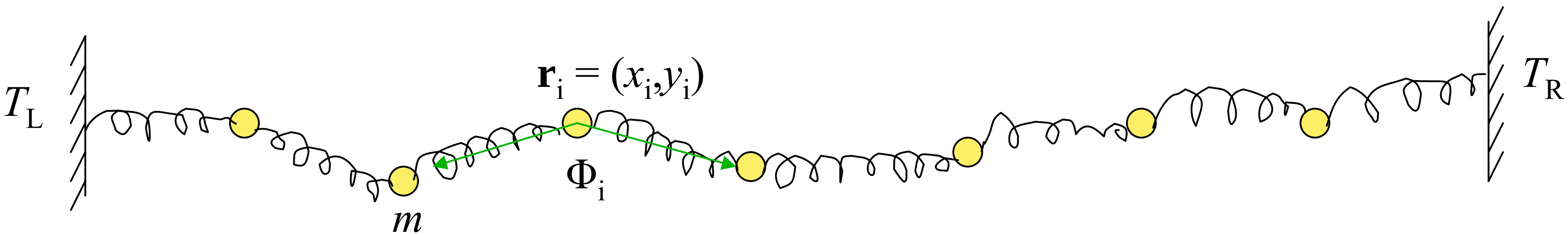

semi-infinite

Junction Part

# Approaches to Heat Transport

| | | |
|---|---|---|
| Molecular dynamics√ /Mode-coupling | Strong nonlinearity | Classical, break down at low temperatures |
| Green-Kubo formula | Both quantum and classical | Linear response regime, apply to junction? |
| Boltzmann-Peierls equation | Diffusive transport | Concept of distribution f($t$,$x$,$k$) valid? |
| Landauer formula√ | Ballistic transport | $T\to 0$, no nonlinear effect |
| Nonequilibrium Green's function √ | A first-principle method | Perturbative. A theory valid for all $T$? |

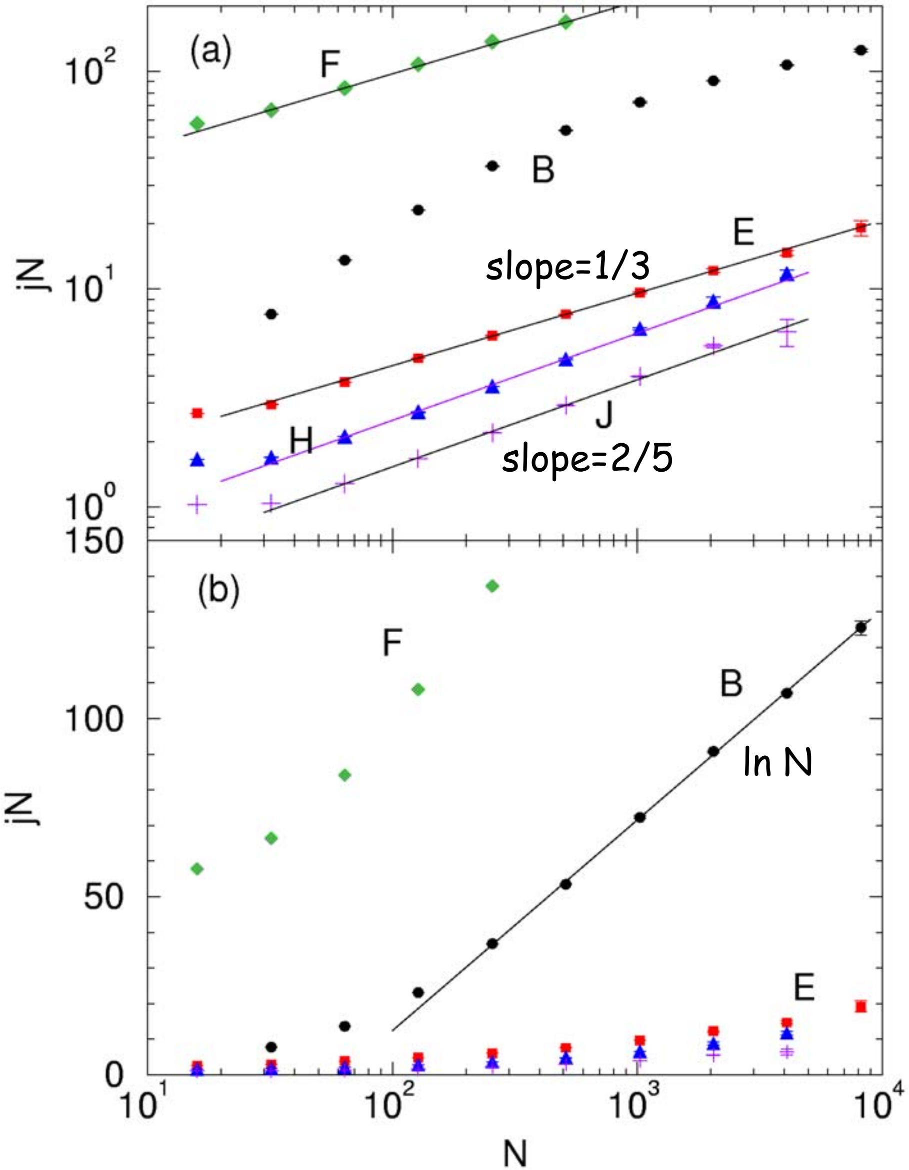
# A Chain Model for Heat Conduction




$$H(\mathbf{p},\mathbf{r}) = \sum_i \left\{ \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} K_r \left( \left| \mathbf{r}_{i+1} - \mathbf{r}_i \right| - a \right)^2 \right\} + K_\Phi \sum_i \cos(\Phi_i)$$

Transverse degrees of freedom introduced

# Conductivity vs Size *N*



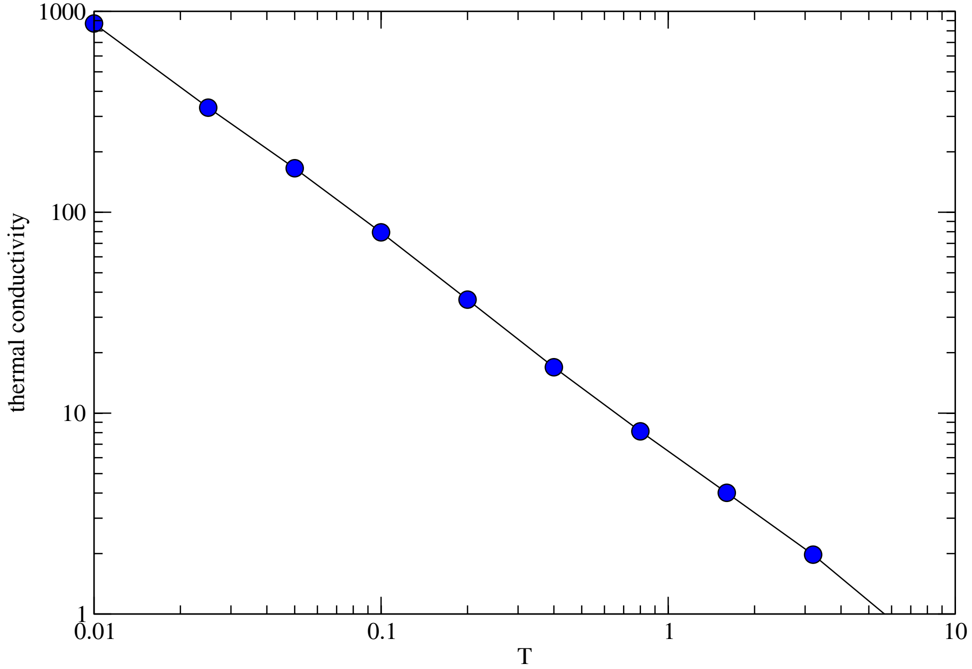

Model parameters ($K_\Phi$, $T_L$, $T_R$):

Set F (1, 5, 7), B (1, 0.2, 0.4), E (0.3, 0.3, 0.5), H (0, 0.3, 0.5), J (0.05, 0.1, 0.2) ,

$m$=1, $a$=2, $K_r$=1.

From J-S Wang & B Li, Phys Rev Lett **92** (2004) 074302; see also PRE **70** (2004) 021204.

# Temperature Dependence of Conductivity in Mode-Coupling Theory



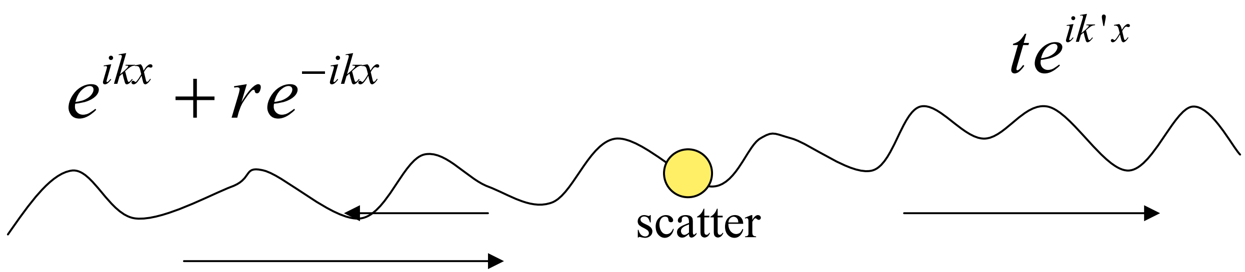

Mode-coupling theory gives a $\kappa \propto 1/T$ behavior for a very broad temperature range. Parameters are for model E with size $L$=8, periodic boundary condition.

J-S Wang, unpublished.

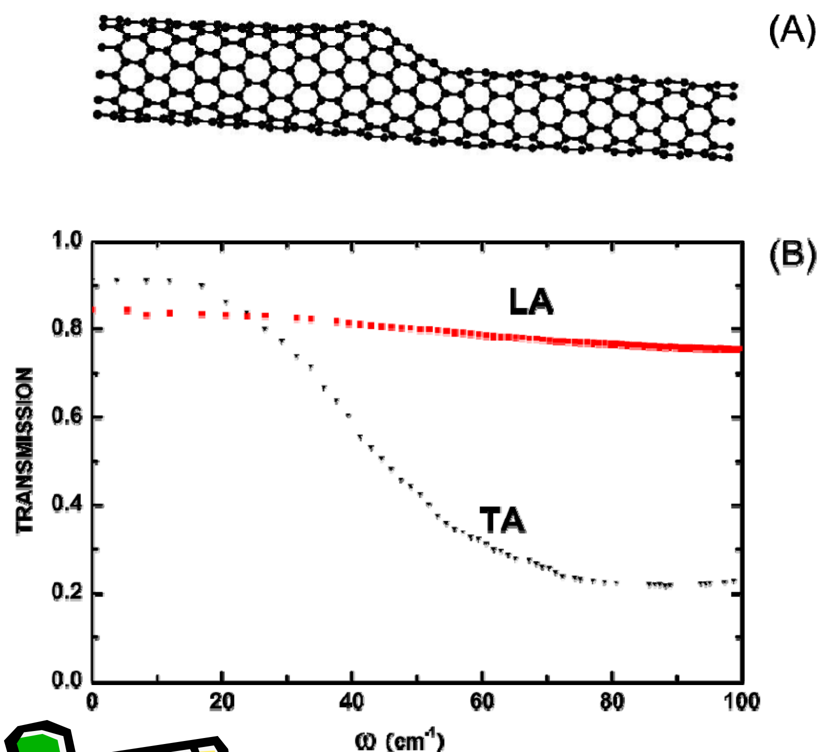
# Ballistic Heat Transport at Low Temperature

- Laudauer formula for heat current

$$I = \frac{1}{2\pi}\int \hbar\omega \,|\, t(\omega)\,|^2 \left(f_L - f_R\right) d\omega$$



# Carbon Nanotube Junction

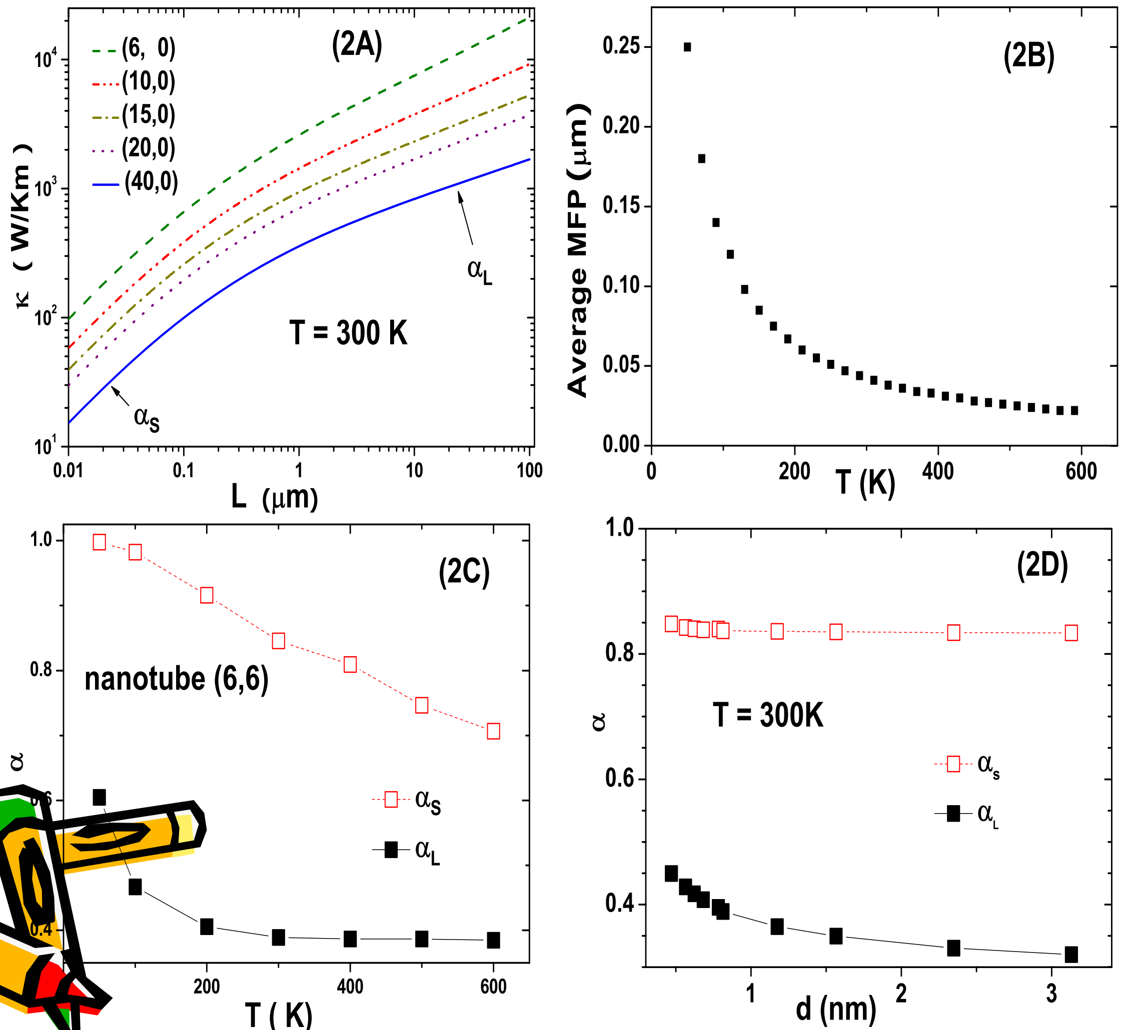



(A) Structure of (11,0) and (8,0) nanotube junction optimized using Brenner potential.

(B) The energy transition coefficient as a function of angular frequency, calculated using a mode-match/singular value-decomposition.

J Wang and J-S Wang, Phys Rev B **74** (2006) 054303.

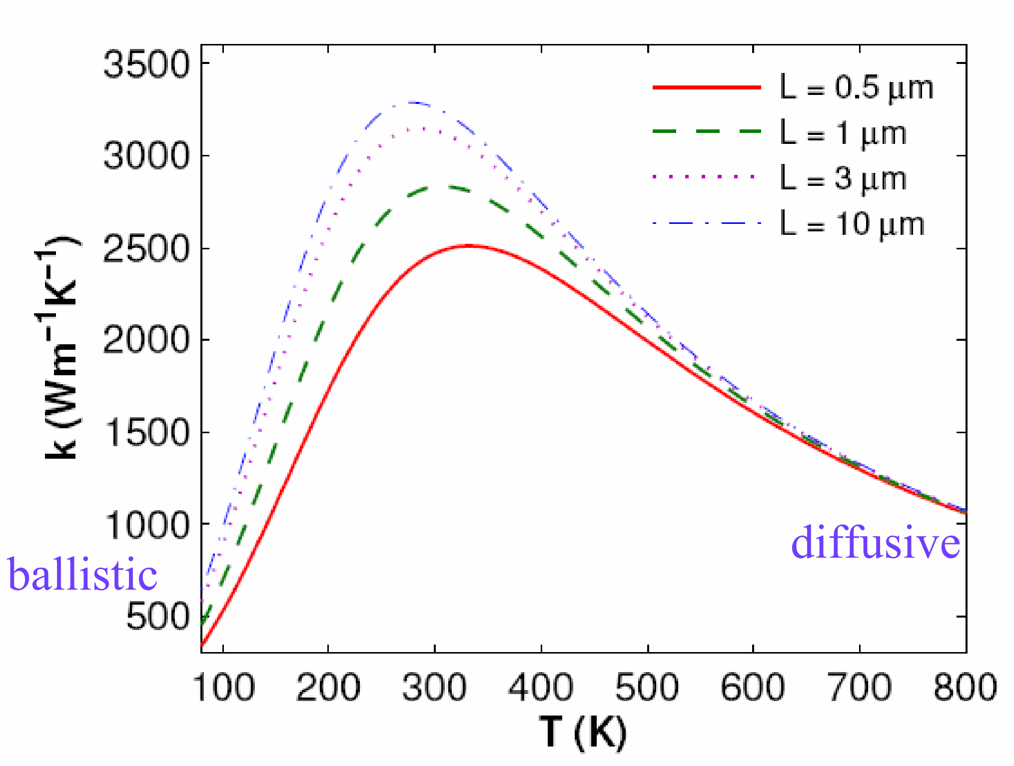
# A Phenomenological Theory for Nonlinear Effect




Assuming $T[\omega] = \ell_0/(\ell_0+L)$, where $\ell_0$ is mean-free path, $L$ is system size. Use Umklapp phonon scattering result $\ell_0 \approx A/(\omega^2 T)$.

From J Wang and J-S Wang, Appl Phys Lett **88** (2006) 111909.

# Experimental Results on Carbon nanotubes




From E Pop, D Mann, Q Wang, K Goodson, H Dai, Nano Letters, **6** (2006) 96.

# Nonequilibrium Green's Function Approach

- Quantum Hamiltonian:

$$H = \sum_{\alpha=L,C,R} H_\alpha + \left(u^L\right)^T V^{LC} u^C + \left(u^C\right)^T V^{CR} u^R + H_n,$$

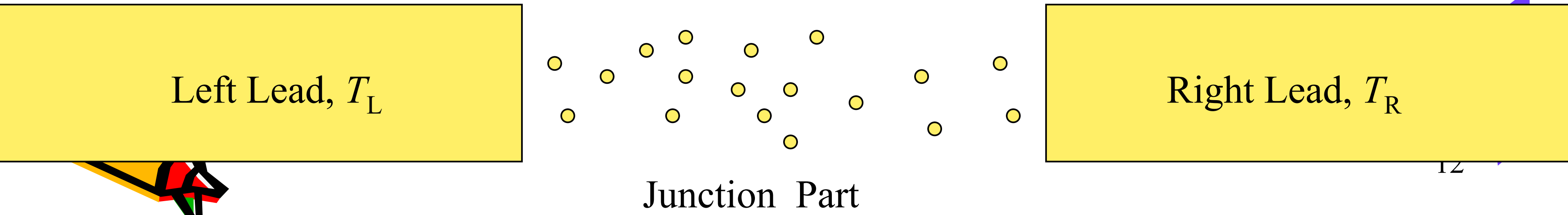
$$H_\alpha = \frac{1}{2}\left(\dot{u}^\alpha\right)^T \dot{u}^\alpha + \frac{1}{2}\left(u^\alpha\right)^T K^\alpha u^\alpha,$$

$$H_n = \frac{1}{3}\sum_{ijk} T_{ijk} u_i^C u_j^C u_k^C$$

$^T$ for matrix transpose

mass $m = 1$,

$\hbar = 1$



# Heat Current

$$I_L = - < \dot{H}_L(t=0) >$$

$$= -\frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{Tr}\left(V^{LC} G^{<}_{CL}[\omega]\right)\omega d\omega$$

$$= -\frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{Tr}\left(G^{r}[\omega]\Sigma^{<}_{L}[\omega] + G^{<}[\omega]\Sigma^{a}_{L}[\omega]\right)\omega d\omega$$

$$\Sigma_L = V^{CL} g_L V^{LC}$$

Where *G* is the Green's function for the junction part, $\Sigma_L$ is self-energy due to the left lead, and $g_L$ is the (surface) green function of the left lead.

# Landauer/Caroli Formulas

- In elastic systems without nonlinear interaction the heat current formula reduces to that of Laudauer formula:

$$I_L = -I_R = \frac{1}{2\pi}\int_0^{\infty} d\omega\, \omega \tilde{T}[\omega]\left(f_L - f_R\right),$$

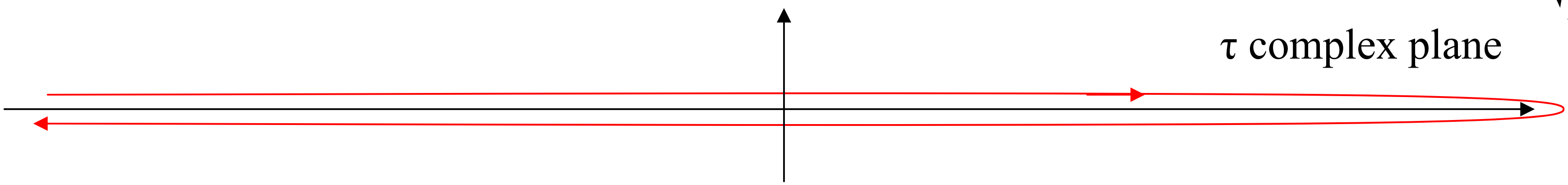
$$\tilde{T}[\omega] = \mathrm{Tr}\left(G^r \Gamma_L G^a \Gamma_R\right),$$

$$\Gamma_\alpha = i\left(\Sigma_\alpha^r - \Sigma_\alpha^a\right),$$

$$f_\alpha = \frac{1}{e^{\hbar\omega/(k_B T_\alpha)} - 1}$$

See, e.g., Mingo & Yang, PRB **68** (2003) 245406.

# Contour-Ordered Green's Functions




$$G(\tau,\tau') = -i < T_\tau u(\tau) u(\tau')^T e^{-i\oint H_n(\tau'')d\tau''} >_0,$$

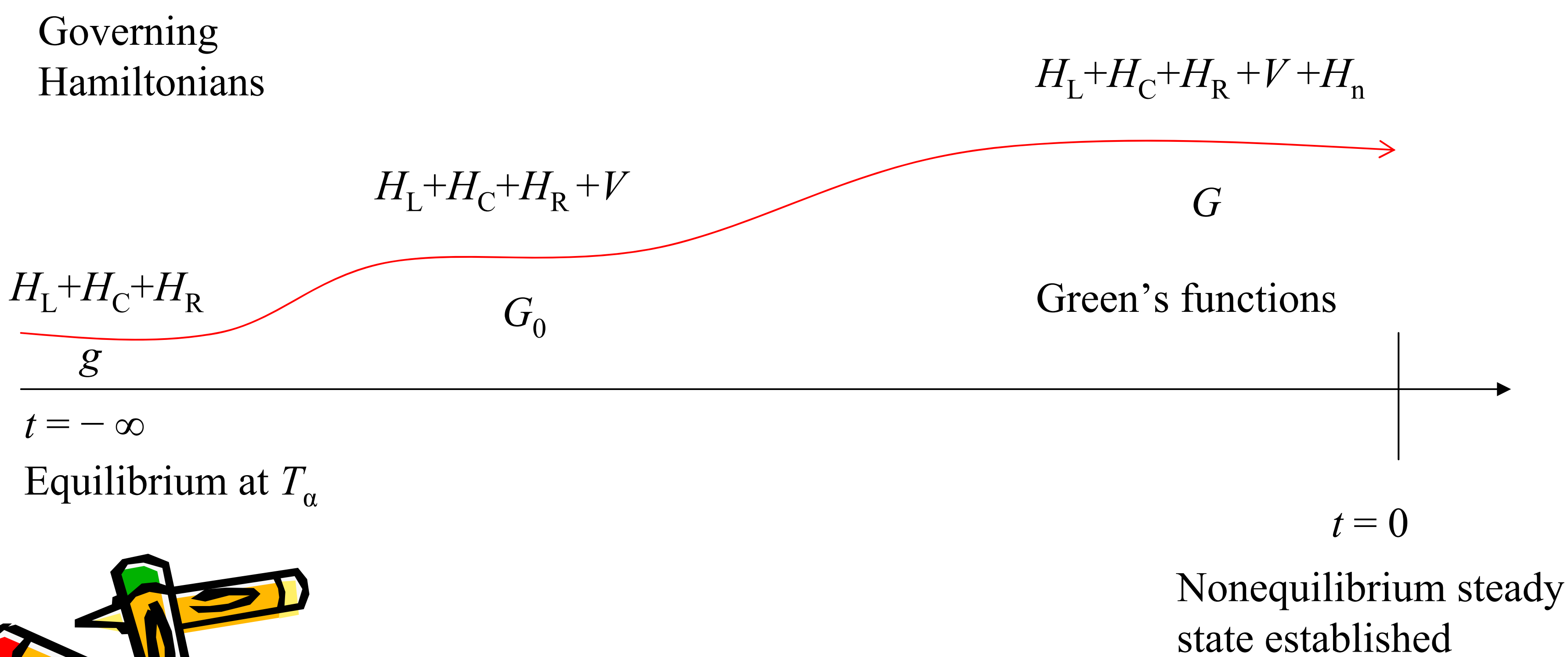
$$G^{\sigma\sigma'}(t,t') = \lim_{\varepsilon\to 0^+} G(t+i\varepsilon\sigma, t'+i\varepsilon\sigma'),$$

$$G^{++} = G^t, \quad G^{+-} = G^<, \quad G^{-+} = G^>, \quad G^{--} = G^{\bar{t}},$$

$$G^r = G^t - G^<, \quad G^a = G^< - G^{\bar{t}}$$

See Keldysh, Meir & Wingreen, or Haug & Jauho

# Adiabatic Switch-on of Interactions



# Contour-Ordered Dyson Equations

$$G_0(\tau,\tau')=g_C(\tau,\tau')+\oint d\tau_1\oint d\tau_2 g_C(\tau,\tau_1)\Sigma(\tau_1,\tau_2)G_0(\tau_2,\tau')$$

$$G(\tau,\tau')=G_0(\tau,\tau')+\oint d\tau_1\oint d\tau_2 G_0(\tau,\tau_1)\Sigma_n(\tau_1,\tau_2)G(\tau_2,\tau')$$

Solution in the frequency domains:

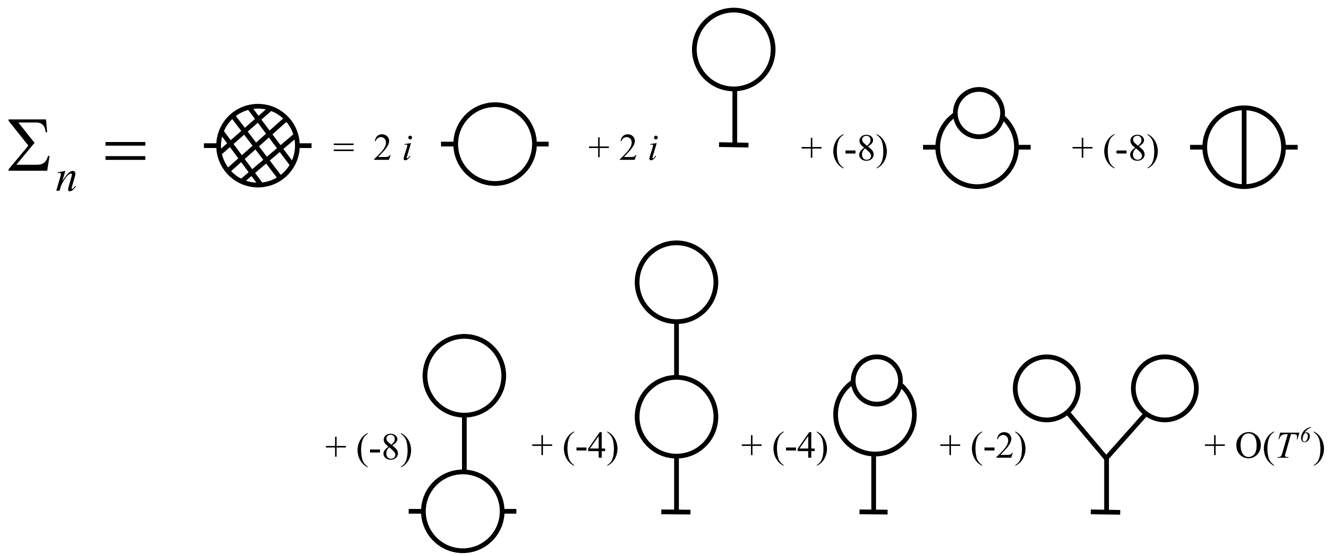
$$G_0^r=\left(G_0^a\right)^\dagger=\frac{1}{(\omega+i\eta)^2-K^C-\Sigma^r},\quad \eta\to 0^+$$

$$G_0^< = G_0^r\Sigma^< G_0^a,$$

$$G^r=\frac{1}{\left(G_0^r\right)^{-1}-\Sigma_n^r},$$

$$G^< = G^r\Sigma_n^< G^a + (I+G^r\Sigma_n^r)G_0^<(I+\Sigma_n^a G^a)$$

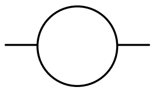
# Feynman Diagrams



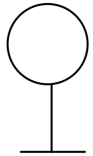

Each long line corresponds to a propagator $G_0$; each vertex is associated with the interaction strength $T_{ijk}$.

# Leading Order Nonlinear Self-Energy

$$\Sigma_{n,jk}^{\sigma\sigma'}[\omega] = 2i \sum_{lmrs} T_{jlm} T_{rsk} \int_{-\infty}^{+\infty} G_{0,lr}^{\sigma\sigma'}[\omega'] G_{0,ms}^{\sigma\sigma'}[\omega - \omega'] \frac{d\omega'}{2\pi}$$



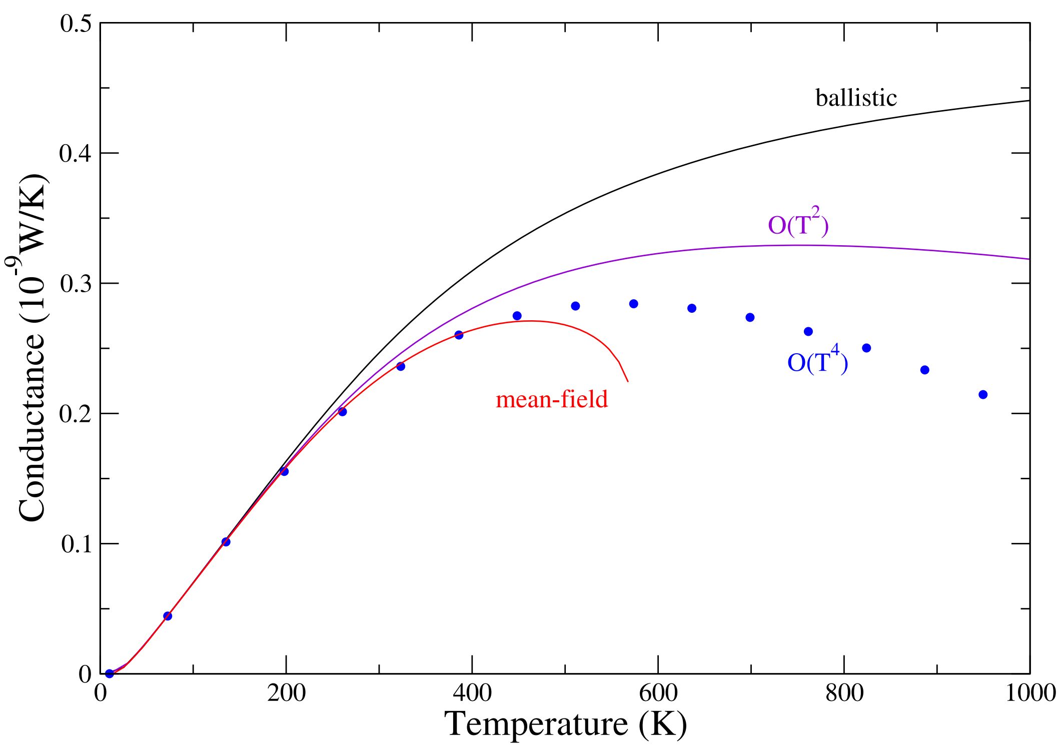
$$+ 2i\sigma\delta_{\sigma,\sigma'} \sum_{lmrs,\sigma''} \sigma'' T_{jkl} T_{mrs} \int_{-\infty}^{+\infty} G_{0,lm}^{\sigma\sigma''}[0] G_{0,rs}^{\sigma''\sigma''}[\omega'] \frac{d\omega'}{2\pi}$$



$$+ O(T_{ijk}^{4})$$

σ = ±1, indices *j*, *k*, *l*, … run over the atom labels

# Three-Atom 1D Junction



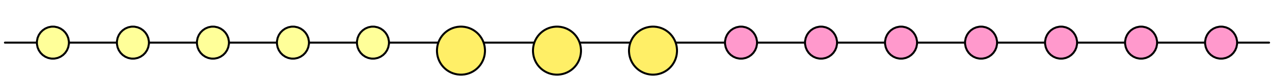

Thermal conductance

$\underline{\kappa} = I/(T_L - T_R)$

From J-S Wang, J Wang, & N Zeng, Phys Rev B **74**, 033408 (2006).

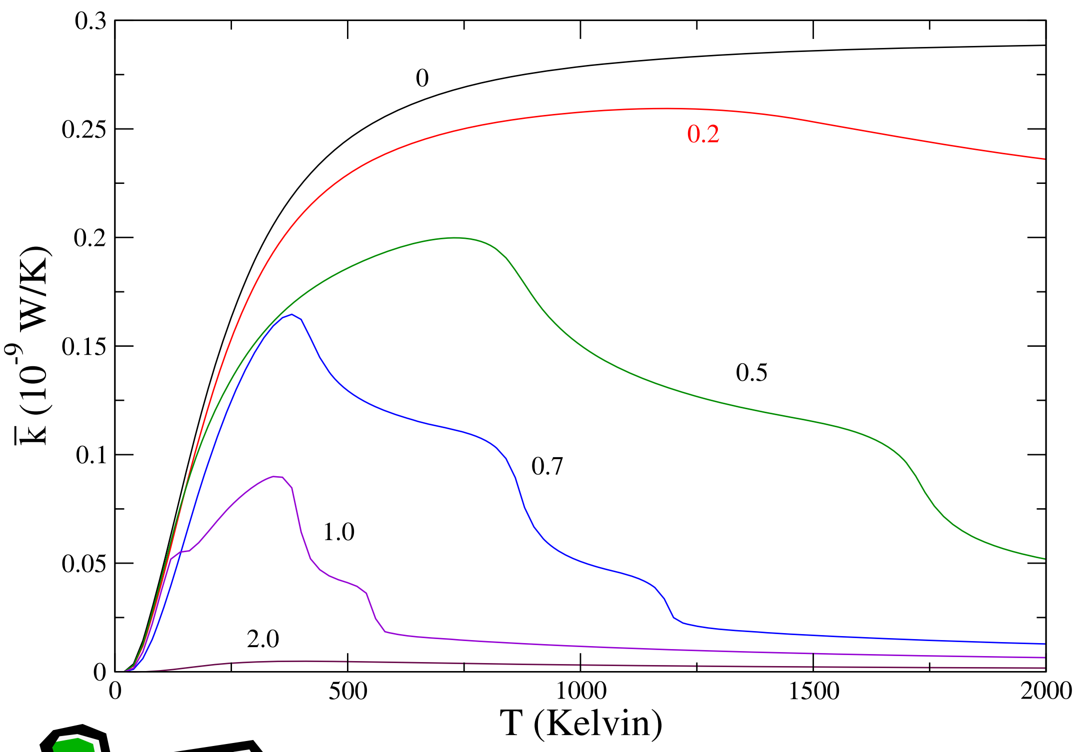
Nonlinear term:

$$\frac{1}{3} t \sum \left(u_j - u_{j+1}\right)^3$$



$k_L$=1.56 $k_C$=1.38, t=1.8 $k_R$=1.44

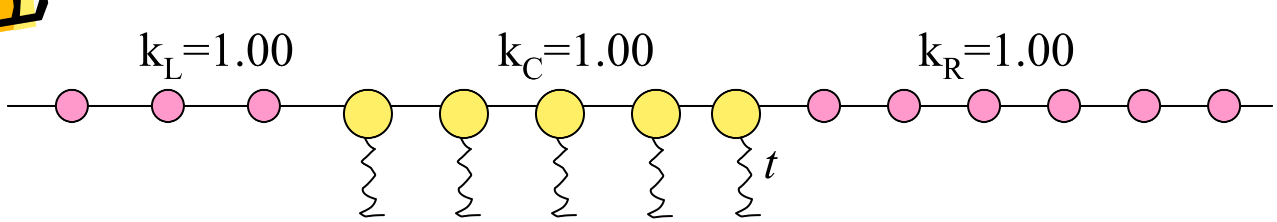
# 1D Cubic On-Site Model



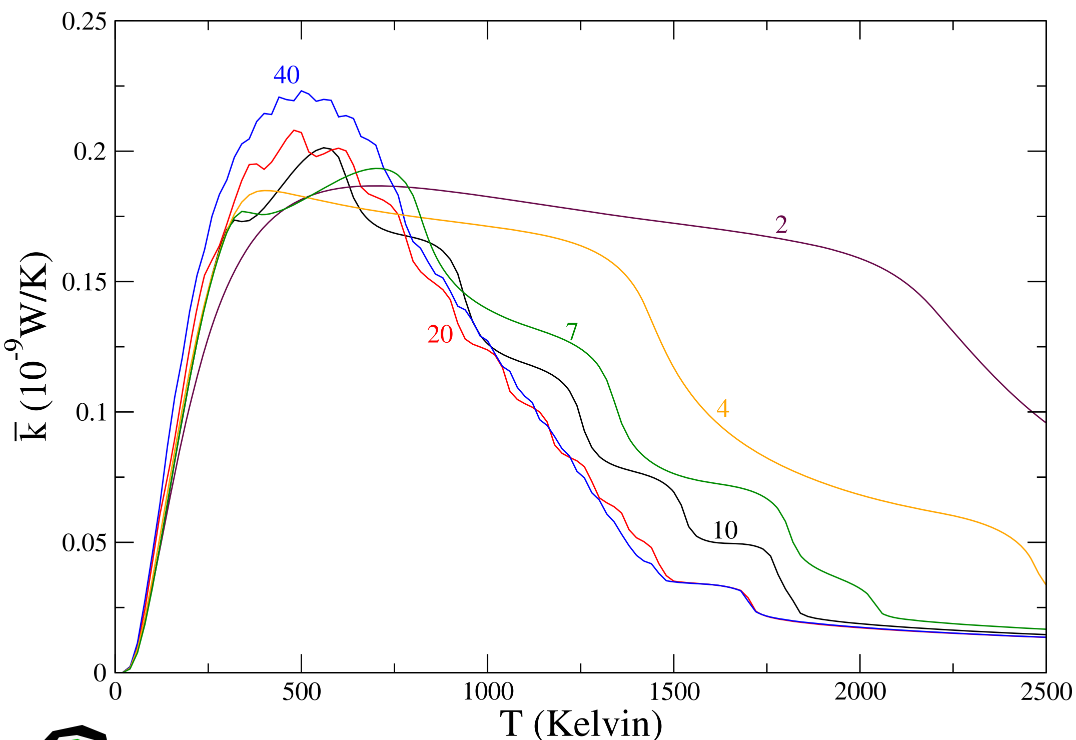

Thermal conductance as a function of temperature for several nonlinear on-site strength $t$. $N$=5. Lowest order perturbation result. J-S Wang, Unpublished.

Nonlinear term:

$$\frac{1}{3} t \sum u_j^3$$



# 1D Cubic On-Site Model

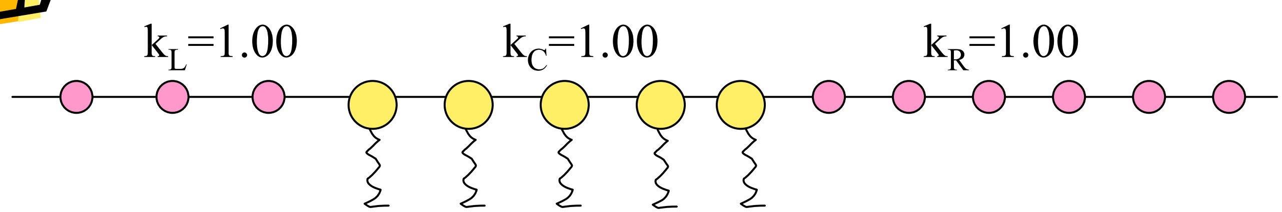



Thermal conductance dependence on chain length *N*. Nonlinear on-site strength *t*= *0.5* [eV/(Å$^3$(amu)$^{3/2}$)].

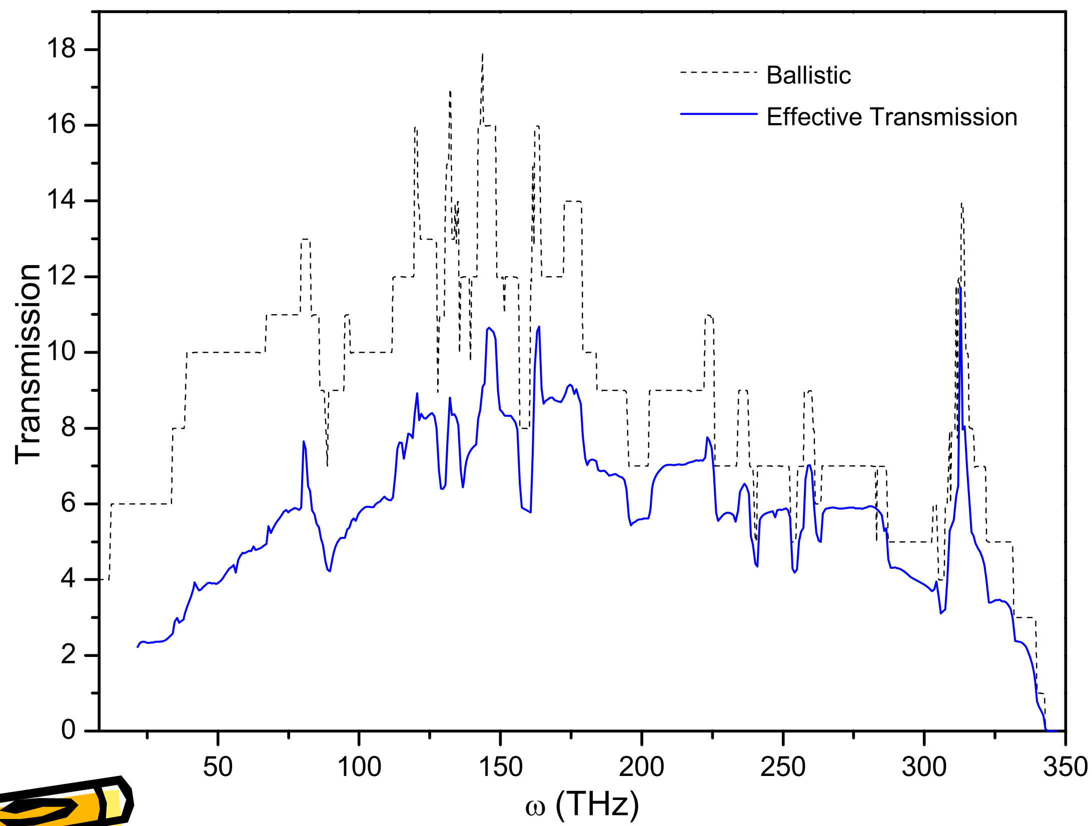
J-S Wang, Unpublished.

Nonlinear term:

$$\frac{1}{3} t \sum u_j^{\,3}$$



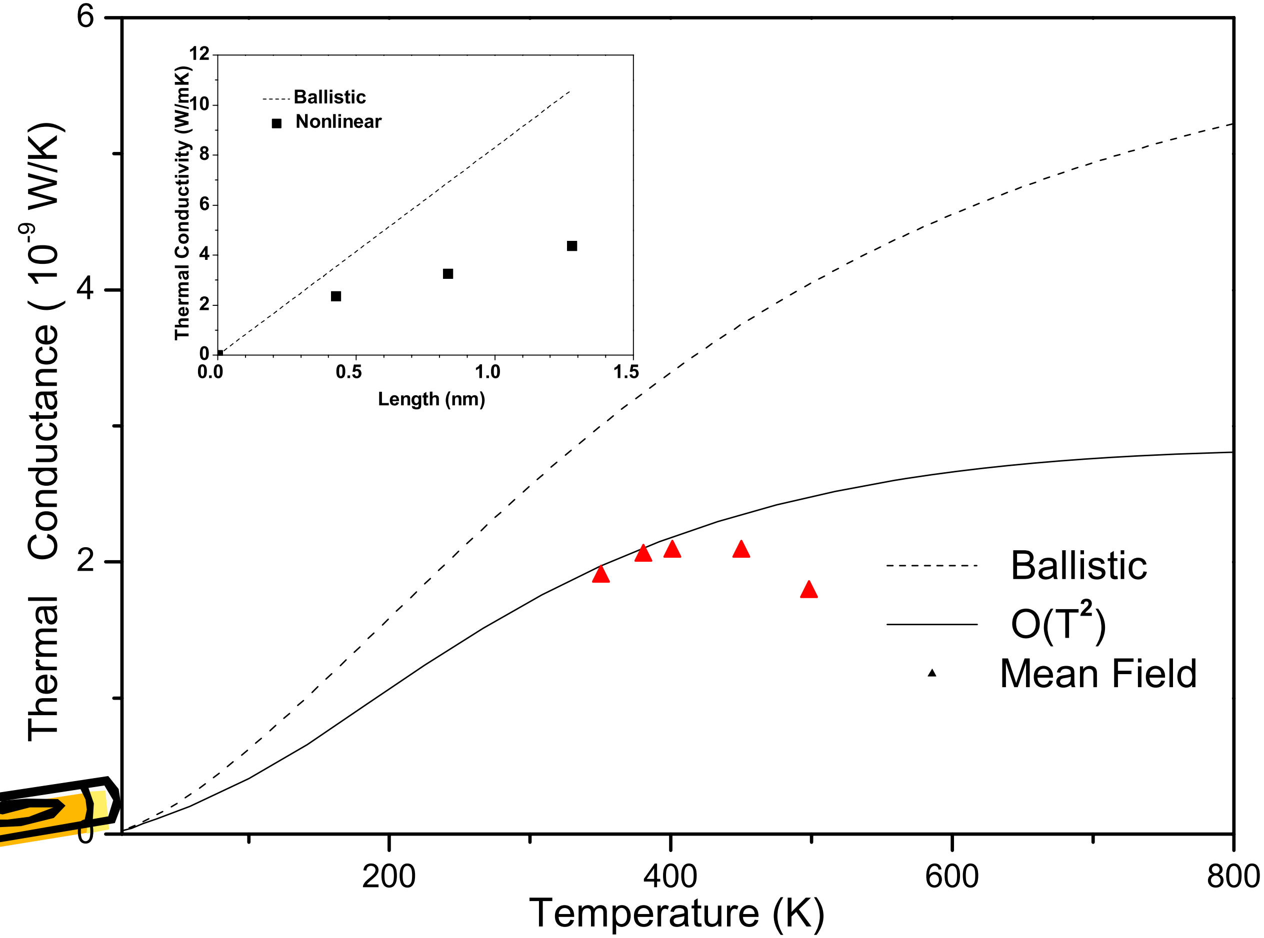
# Nanotube Energy Transmissions




The transmissions in a one-unit-cell carbon nanotube junction of (8,0) at 300 Kelvin.

Phys Rev B **74**, 033408 (2006).

# Thermal Conductance of Nanotube Junction




Phys Rev B **74**, 033408 (2006).

# Conclusion

- The nonequilibrium Green's function method is promising for a truly first-principle approach. Appears to give excellent results up to room temperatures.
- Still too slow for large systems.
- Need a better approximation for self-energy.