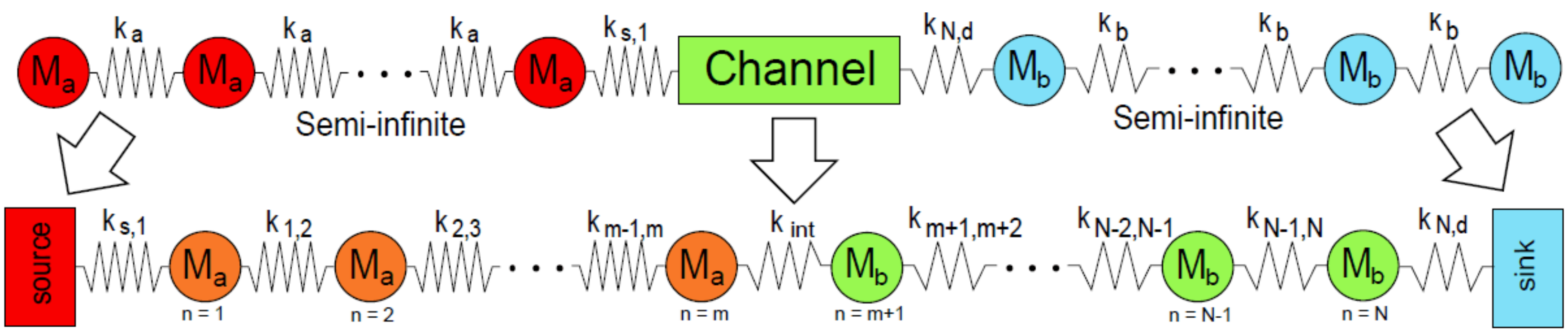
SAND2011-6872C

# 1D Non-Equilibrium Green's Functions

- Green's functions are a mathematical method for solving linear, inhomogeneous differential equations subject to specific initial and boundary conditions
- The system is described by a harmonic Newtonian system of equations
- We apply the method to calculate frequency dependent phonon transmission
- The source and sink are semi-infinite 1-D "bulk" materials
- The channel is explicitly described by a system of *N* coupled equations
- We investigate the effect of changing (1) impurity mass, (2) interface bonding, and (3) both, by reducing the channel to only include the feature of interest

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## Slide 1

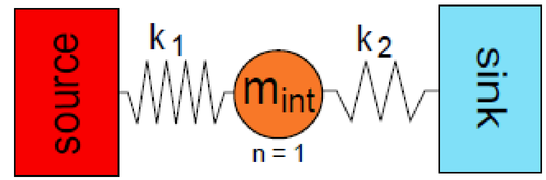
**PN1** here is no mention on this slide of an impurity mass but we go directly to an optimal impurity mass on the next slide?

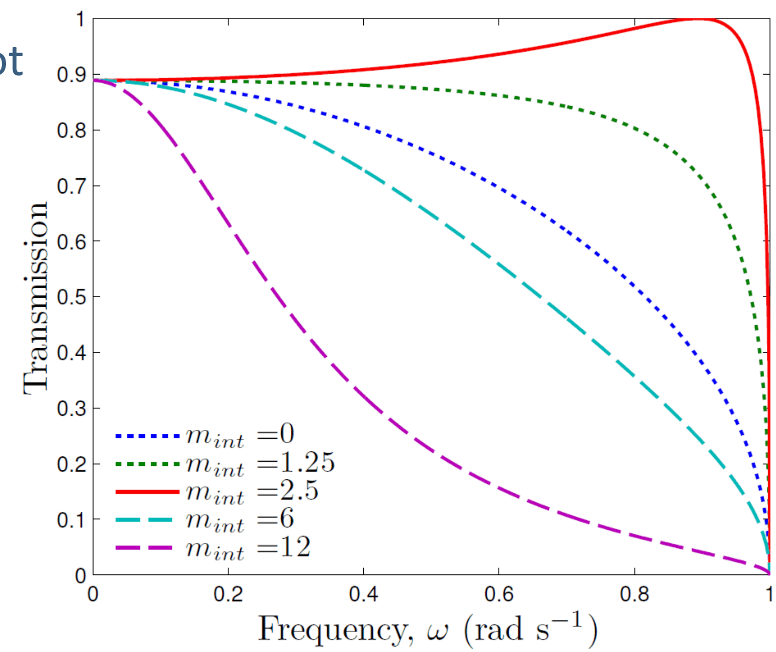
Pamela Norris, 9/9/2011

# Effect of Interface Impurity Mass

- Impurity mass which yields the maximum transmission is independent of spring constants on either side of the interface
- Maximizes all frequencies simultaneously
- When $m_{int}$ goes to zero, transmission does not go to zero
- As $m_{int}$ goes to infinity, transmission goes to zero, but at different rates for different frequencies

$$m_{int,max} = \frac{m_1 + m_2}{2}$$

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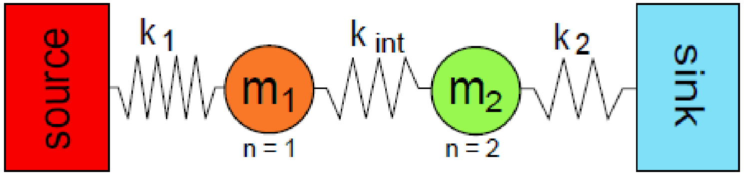
## Slide 2

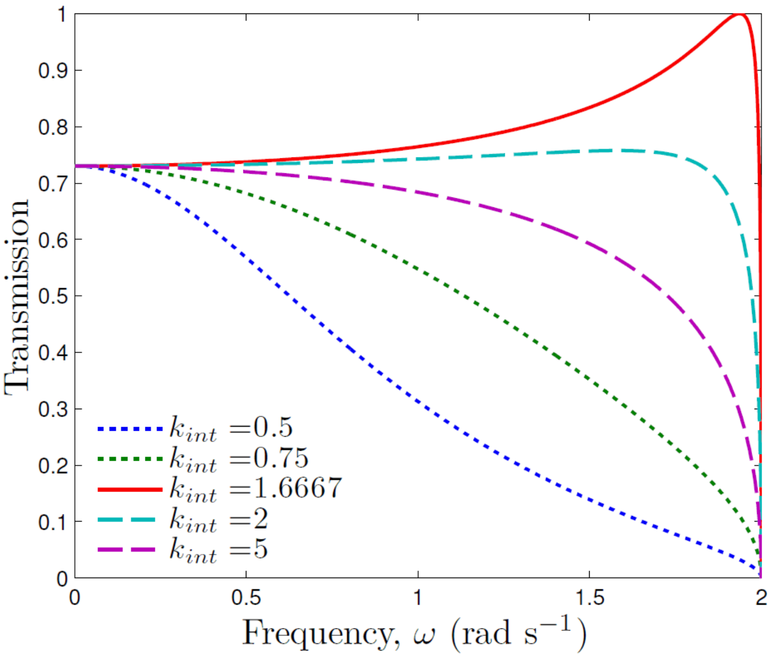
**PN2** following up on comment from last slide---we need to introduce the impurity mass
Pamela Norris, 9/9/2011

# Effect of Interface Adhesion

- Interface adhesion which yields the maximum transmission is independent of mass and frequency
- All frequencies are maximized for the same choice of $k_{int,max}$
- As $k_{int}$ goes to zero so does the transmission
- As $k_{int}$ goes to infinity transmission does not go to a maximum

$$k_{int,max} = \frac{2k_1 k_2}{k_1 + k_2}$$

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# Simultaneous Effects

- Choice of interface adhesion and mass depends on temperature regime at which the device will be operated

$$k_{int,max} = f(m_{int}, \omega) \qquad m_{int,max} = f(k_{int}, \omega)$$

$$k_{int,max} = \frac{-2k_2 m_2 (k_1 m_1 + m_{int}(m_{int} - m_1)\omega^2)}{-k_1 m_1 m_2 + k_2 m_2 (m_1 - 2m_{int}) + m_{int}(m_1 - m_{int})}$$

$$m_{int,max} = \frac{k_2 m_2 (2k_{int} + m_1 \omega^2) - k_{int}(k_{int}(m_2 - m_1) + m_1 m_2 \omega^2)}{2(k_2 m_2 \omega^2 + k_{int}^2 - k_{int} m_2 \omega^2)}$$