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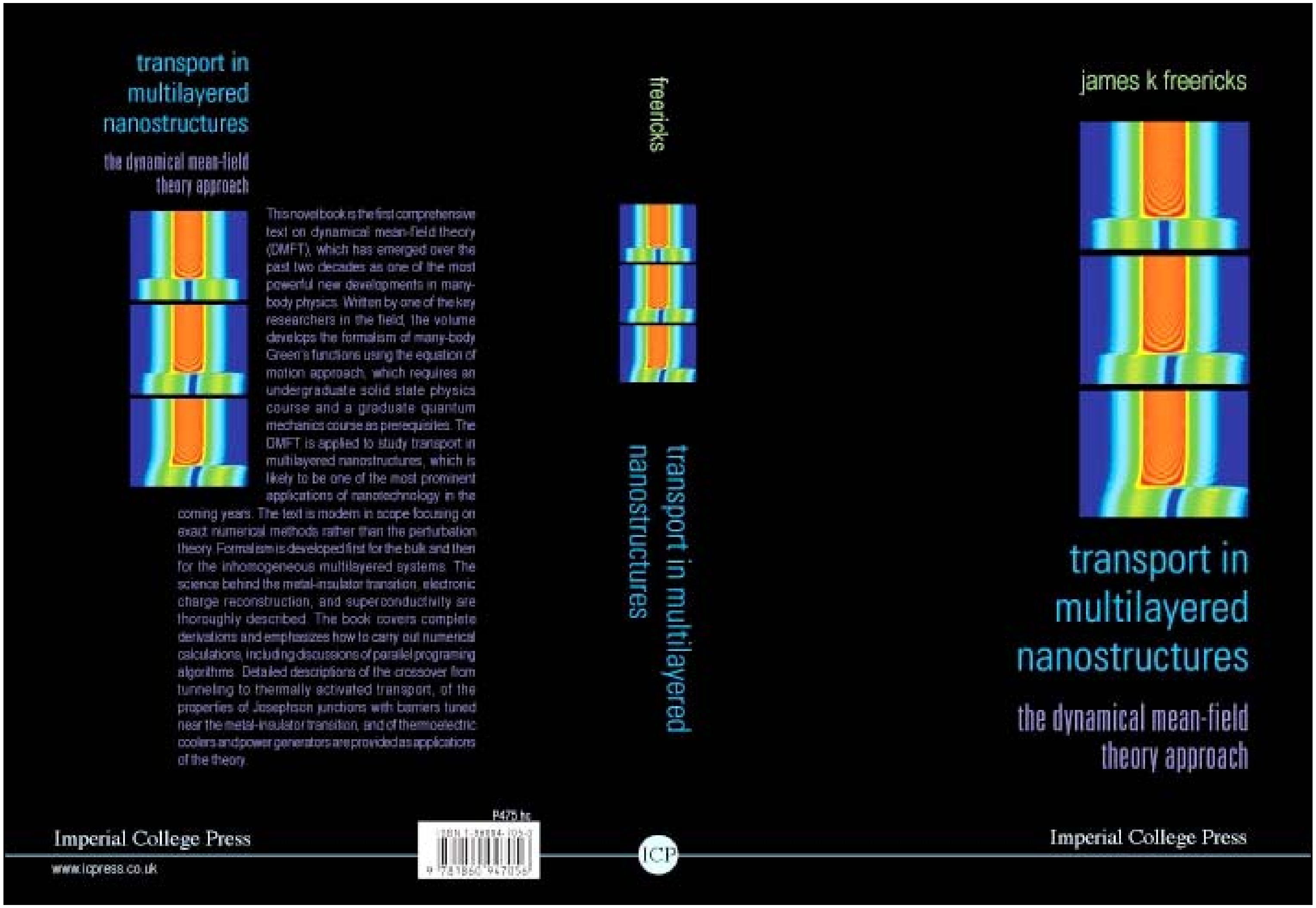
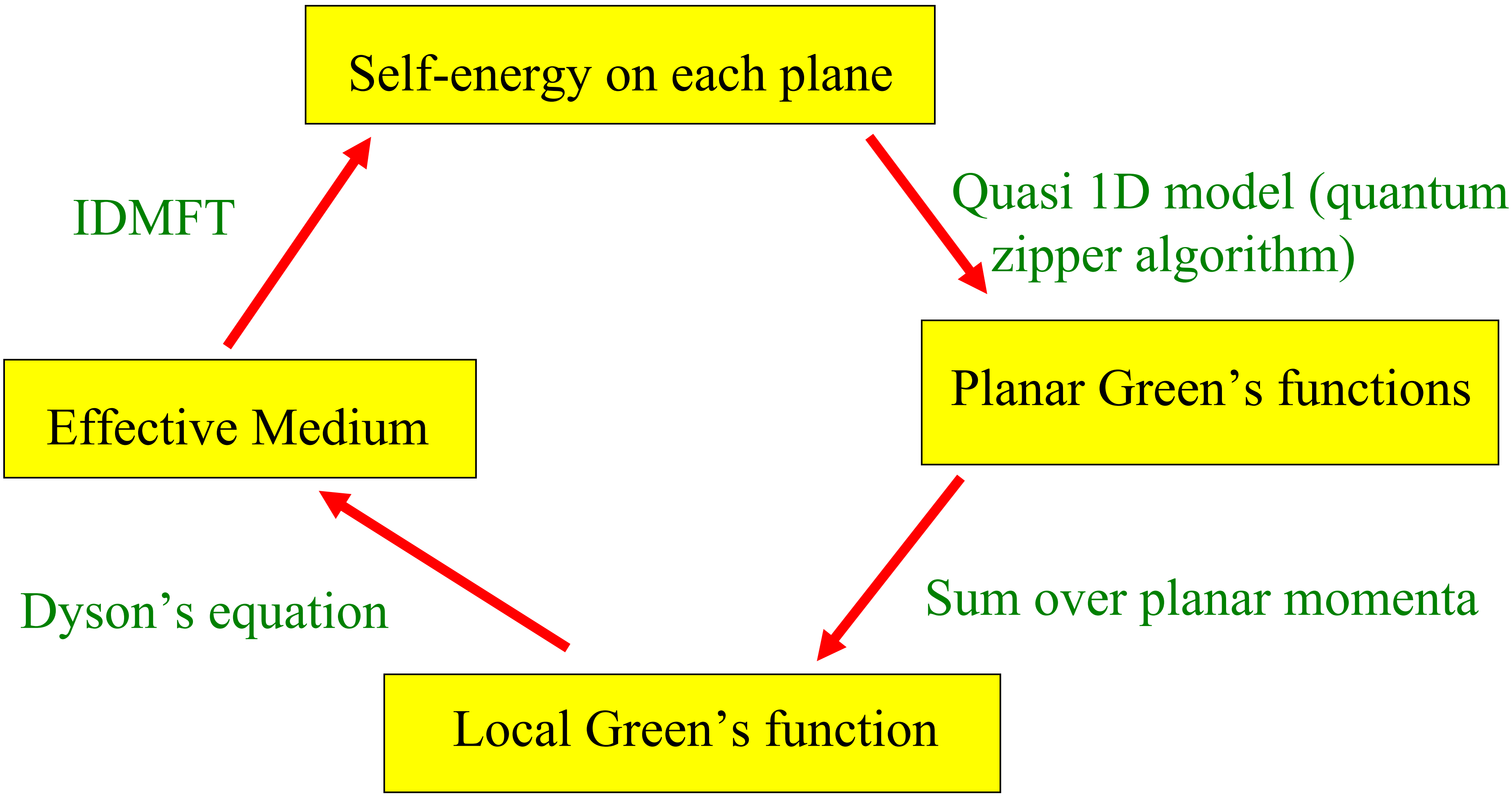


Computational Algorithm



Algorithm is iterated until a self-consistent solution is achieved

Charge transport …

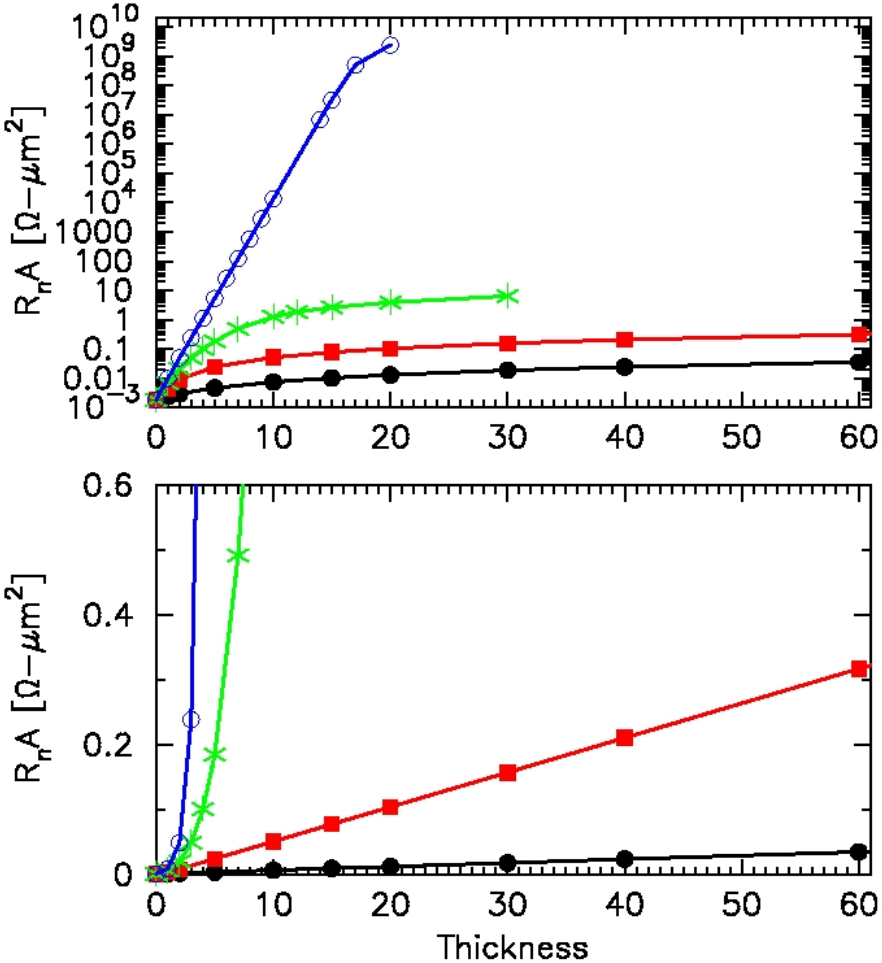
Junction resistance

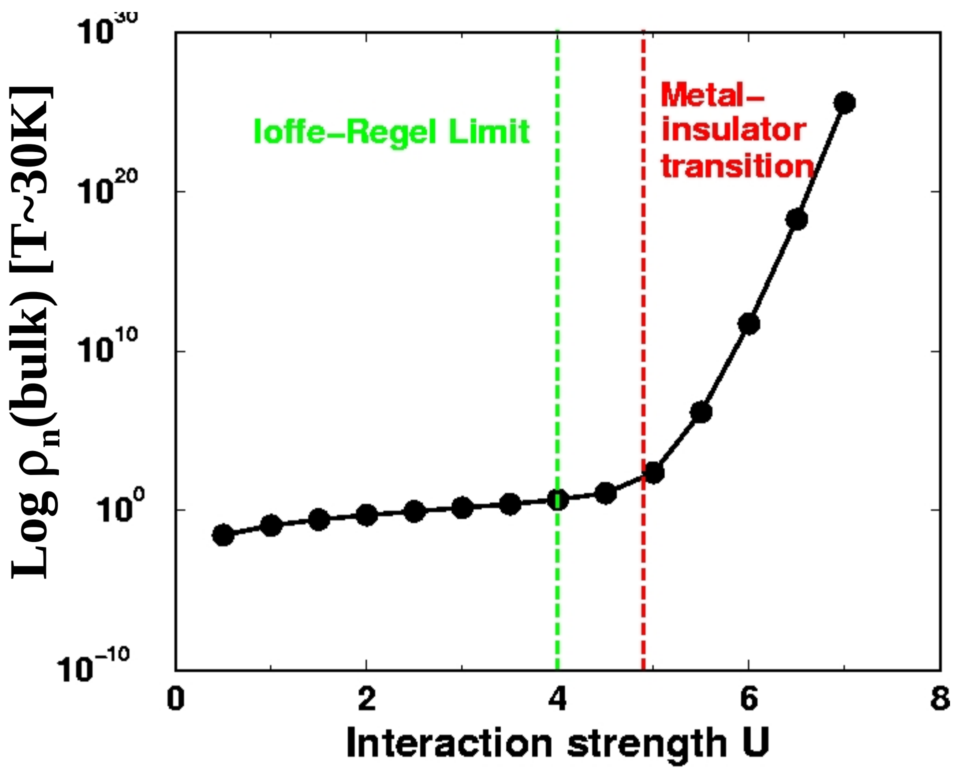
- The linear-response resistance can be calculated in equilibrium using a Kubo-Greenwood approach.
- We must work in real space because there is no translational symmetry.
- R_n is calculated by inverting the isothermal conductivity matrix and summing all matrix elements of the inverse.

Junction resistance (derivation)

- Maxwell's equation gives $\mathbf{j}_i=\sum_j\sigma_{ij}\mathbf{E}_j$ where the index denotes a plane in the layered device. (The field at plane j causes a current at plane i.)
- Taking the matrix inverse gives $\mathbf{E}_i=\sum_j\sigma^{-1}_{ij}\mathbf{j}_j$; but the current is conserved, so **j** does not depend on the planar index.
- Calculating the voltage gives $V=a\sum_i E_i=a\sum_{ij}\sigma^{-1}_{ij}j$, so the resistance-area product is $R_nA=a\sum_{ij}\sigma^{-1}_{ij}$

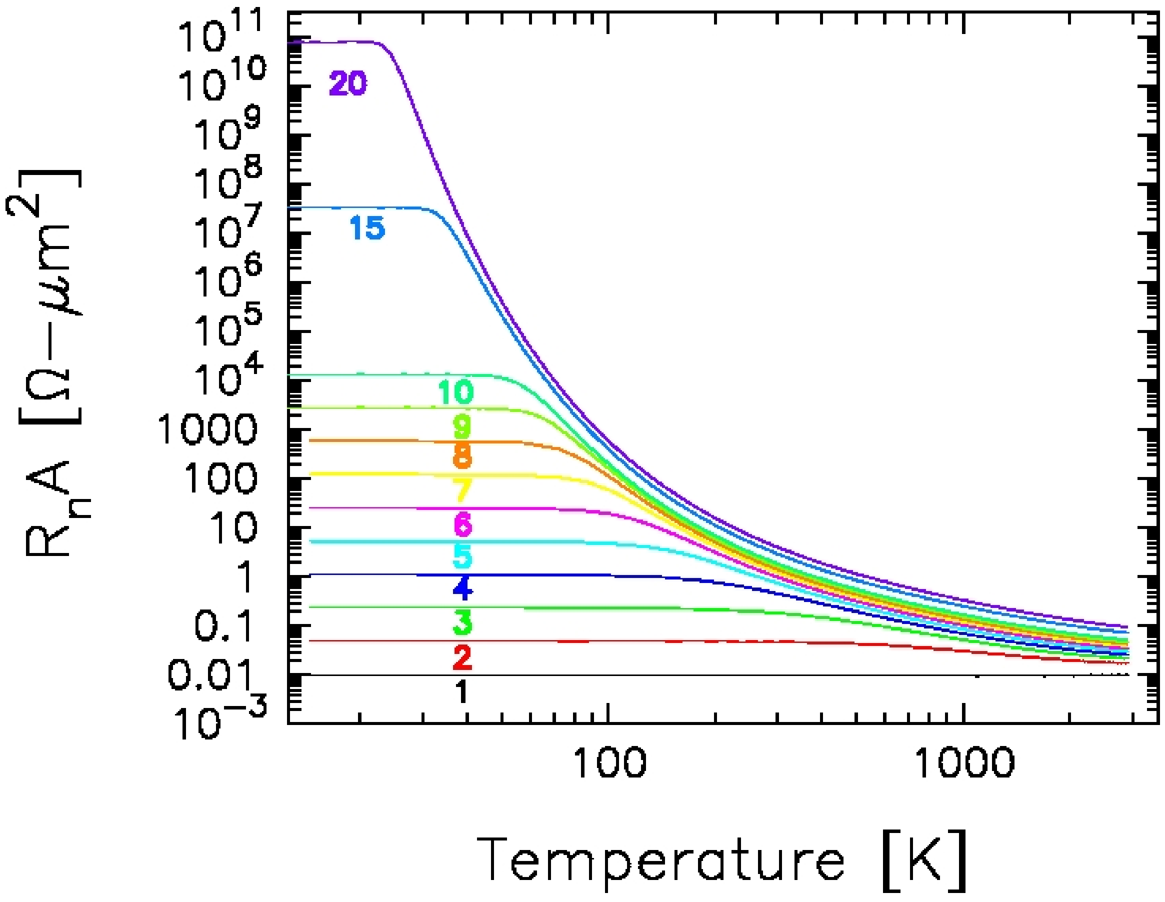
Resistance versus resistivity





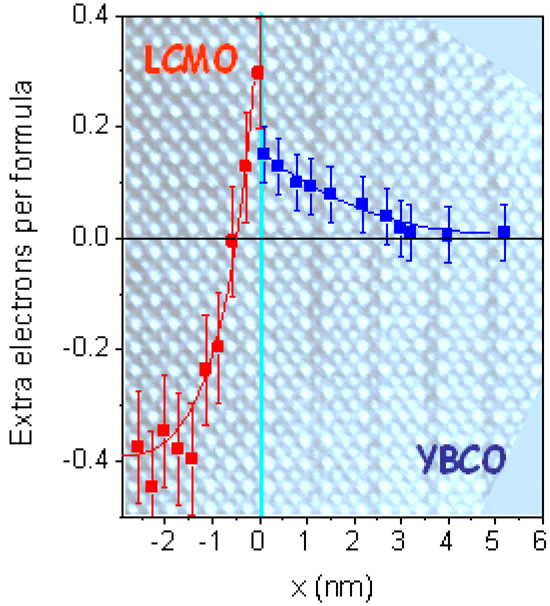
Resistance for U=6 (correlated insulator)

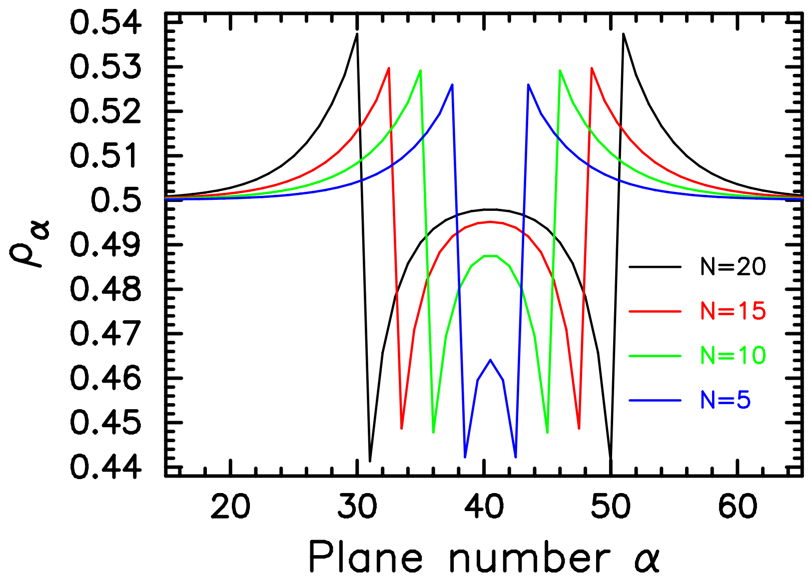
Resistance here shows the tunneling plateaus clearly, and a strong temperature dependence in the incoherent regime.



Particle-hole asymmetry is necessary for thermoelectric devices …

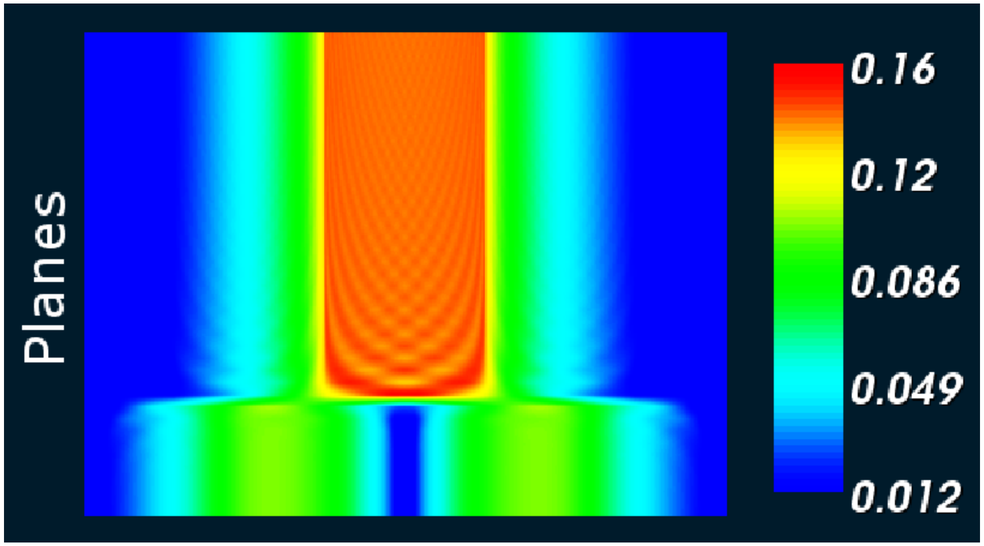
Electronic charge reconstruction



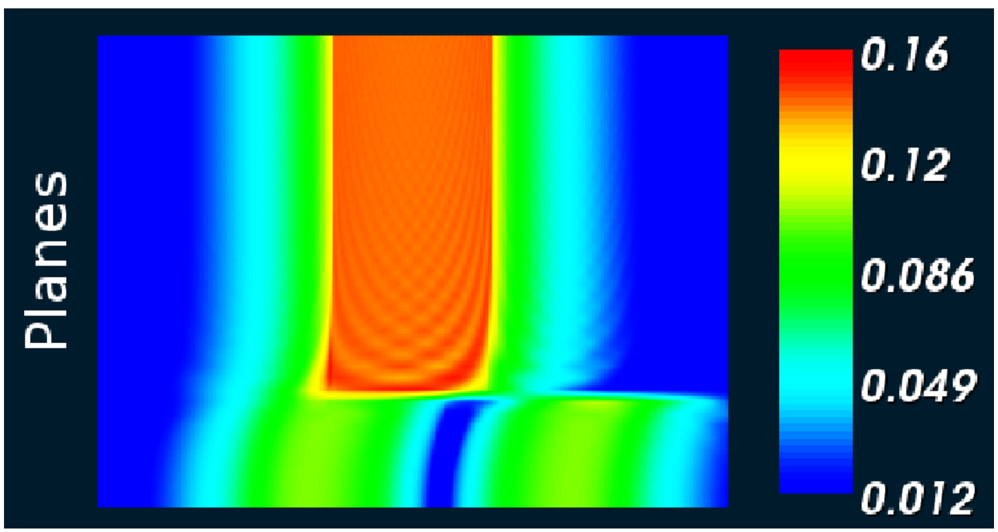


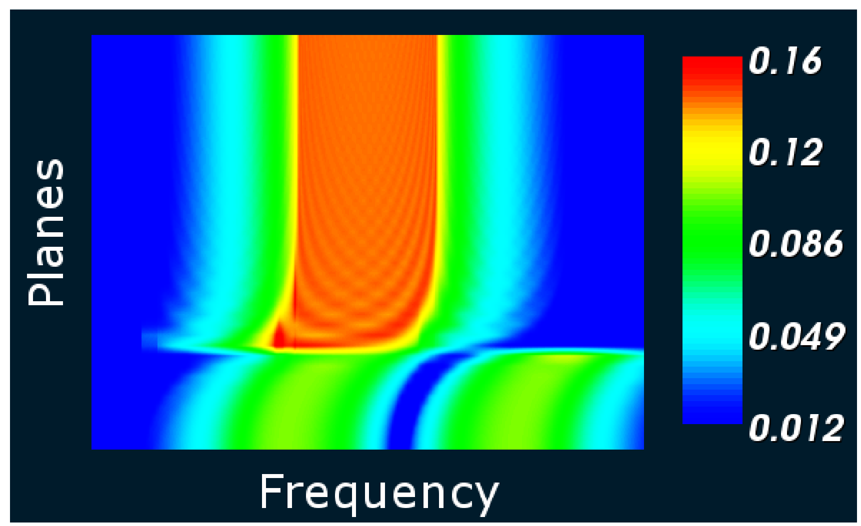
Using a scanning transmission electron microscope with electron energy-loss spectroscopy, one can directly measure the electronic charge at each plane of a strongly correlated multilayered nanostructure. Left are experimental results by Varela et al. on YBCO/LCMO heterostructures, right is a simple theory for a correlated nanostructure.

DOS with electronic charge reconstruction



Changing the band offsets creates particle-hole asymmetry in the DOS.





Thermal transport in a multilayered nanostructure

Heat Current Conservation

- Unlike the charge current, the heat current need not be conserved in a multilayered nanostructure.
- The experimental conditions will determine the boundary conditions for the heat current, which need to be employed to solve for the heat transport.
- We describe the Seebeck effect here.

Heat transport equations

In the presence of field and temperature gradients, the charge and heat currents satisfy:

$$j_i=e^2\sum_j L^{11}_{ij} E_j - e \sum_j L^{12}_{ij} (T_{j+1}-T_{j-1})/2a$$

$$j_{Qi}=\sum_j L^{21}_{ij} E_j - \sum_j L^{22}_{ij} (T_{j+1}-T_{j-1})/2a$$

Where the L matrices are found from the **Jonson-Mahan theorem** (current and heat-current correlation functions in real space)

Seebeck effect

In the Seebeck effect, we isolate the device and work with an open circuit. *Hence there is no heat created or destroyed in the steady state (i.e., the heat current is conserved) and the total charge current vanishes*:

The E field becomes $E_j = \sum_{jk} (L^{11})^{-1}_{ij} L^{12}_{jk} (T_{k+1} - T_{k-1})/2a$

The temperature gradients become

$\sum_j M^{-1}_{ij} j_Q = -(T_{i+1} - T_{i-1})/2a$; $M = -L^{21}(L^{11})^{-1}L^{12} + L^{22}$

Hence, $\Delta T = -\sum_{ij} M^{-1}_{ij} j_Q$, $\Delta V = -a\sum_{ij}[(L^{11})^{-1}L^{12}M^{-1}]_{ij} j_Q$, and the Seebeck coefficient is

$$S = \Delta V/\Delta T = a\sum_{ij}[(L^{11})^{-1}L^{12}M^{-1}]_{ij} / \sum_{ij} M^{-1}_{ij}$$

Note the weighting by the matrix M, which is different for a nanostructure than in the bulk, where that factor cancels as can be seen from the convolution theorem!

Thermal transport created from electronic charge reconstruction

Seebeck effect

Numerically we evaluate the Seebeck coefficient for two particle-hole symmetric bulk materials with an electronic charge reconstruction. **The Seebeck effect can become quite large!**

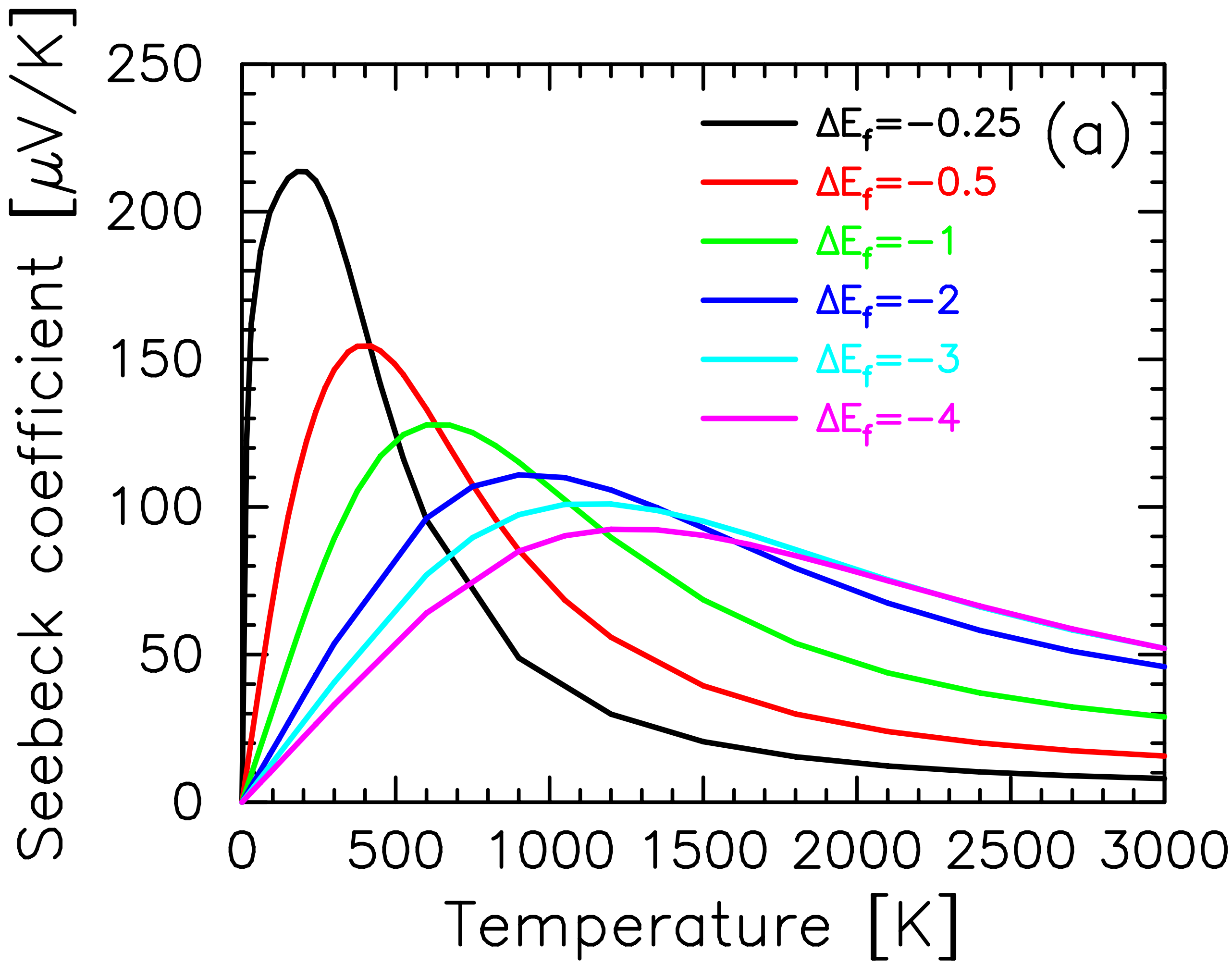


Figure of merit

The figure-of-merit can also become large, and **is bigger than 1 for small band offsets**. The phonon thermal conductance can dramatically reduce the figure-of-merit though.