

General iterative lead self-energy

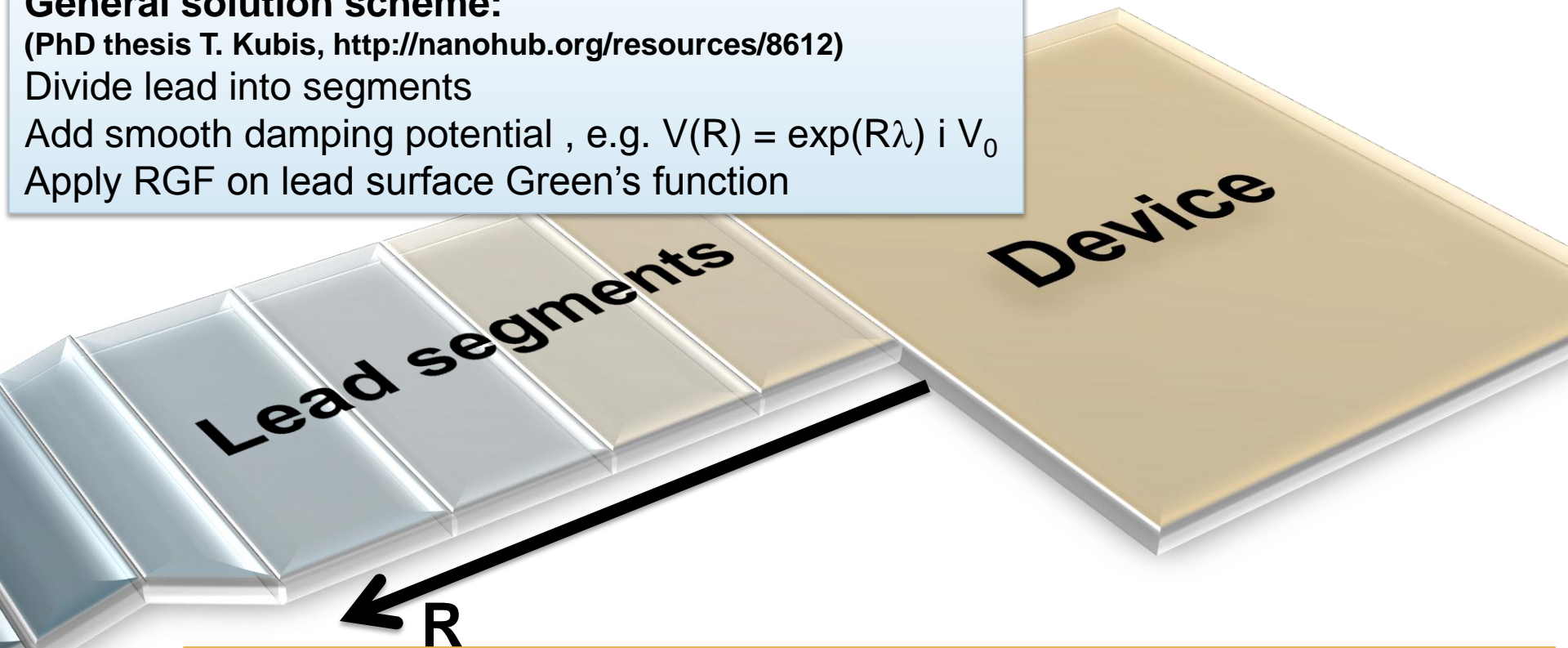
General solution scheme:

(PhD thesis T. Kubis, <http://nanohub.org/resources/8612>)

Divide lead into segments

Add smooth damping potential , e.g. $V(R) = \exp(R\lambda) i V_0$

Apply RGF on lead surface Green's function



Compared to Sancho-Rubio and Transfer Matrix Method:

- Comparable in speed with Sancho-Rubio
- Completely general approach (dimensions, Hamiltonian, lead structure...)
- Requires incoherent scattering to speed up convergence