Using Filon Integration for Perovskite Superlattice Calculations

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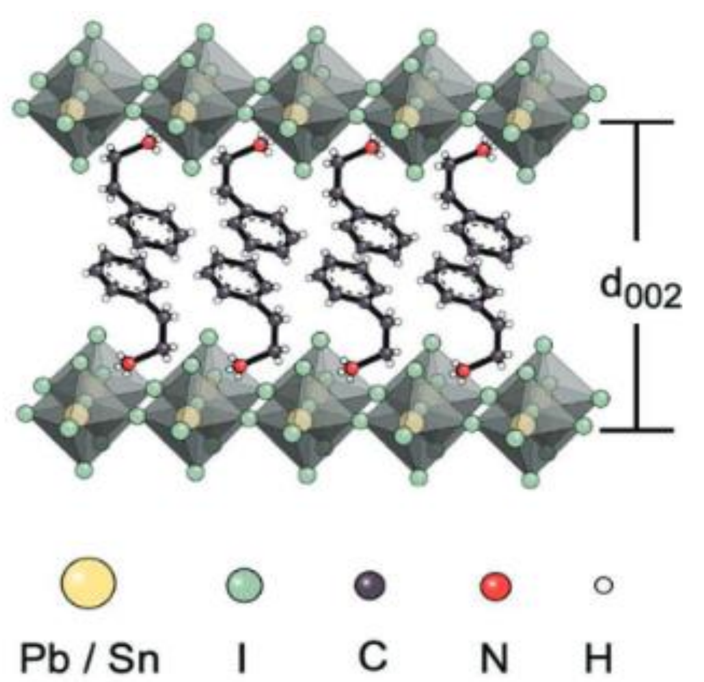
Abstract

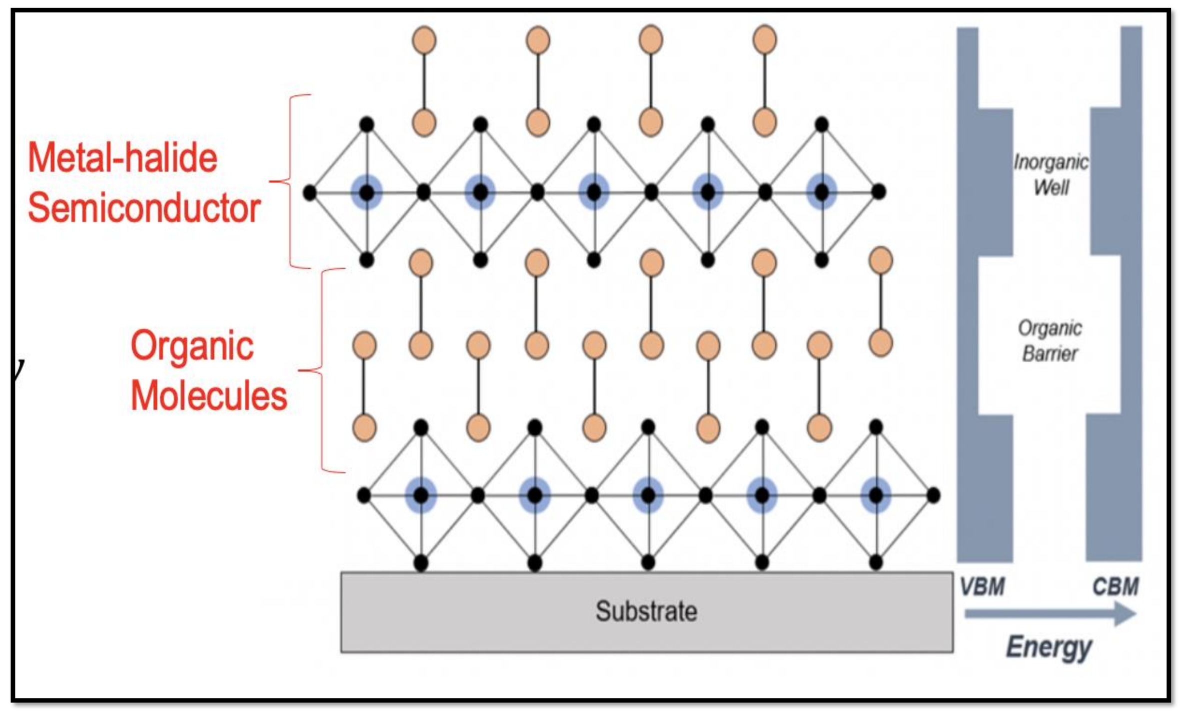
Perovskites electronic properties can be better understood using a superlattice model and the Schrodinger's equation. V(ρ) is calculated using Filon's method and cubic fits gives results within 0.2% of truth.

Background

- Perovskites are a type of semiconductor that is widely studied and used for solar panels.
- Many 2D perovskites have layers of organic materials (carbon based) and inorganic materials (metal based).
- These different layers can be treated as a well (sinkhole) or a barrier (wall) for electrons.
- An alternating well and barrier system is called a superlattice.
- The Colton research group experiments on these materials to obtain their electronic structure characteristics (i.e. band gap).
- To better understand these perovskites, we can numerically calculate what the electronic properties will be depending on a few input variables.
- In our research we want to change these variables to predict the electronic properties.



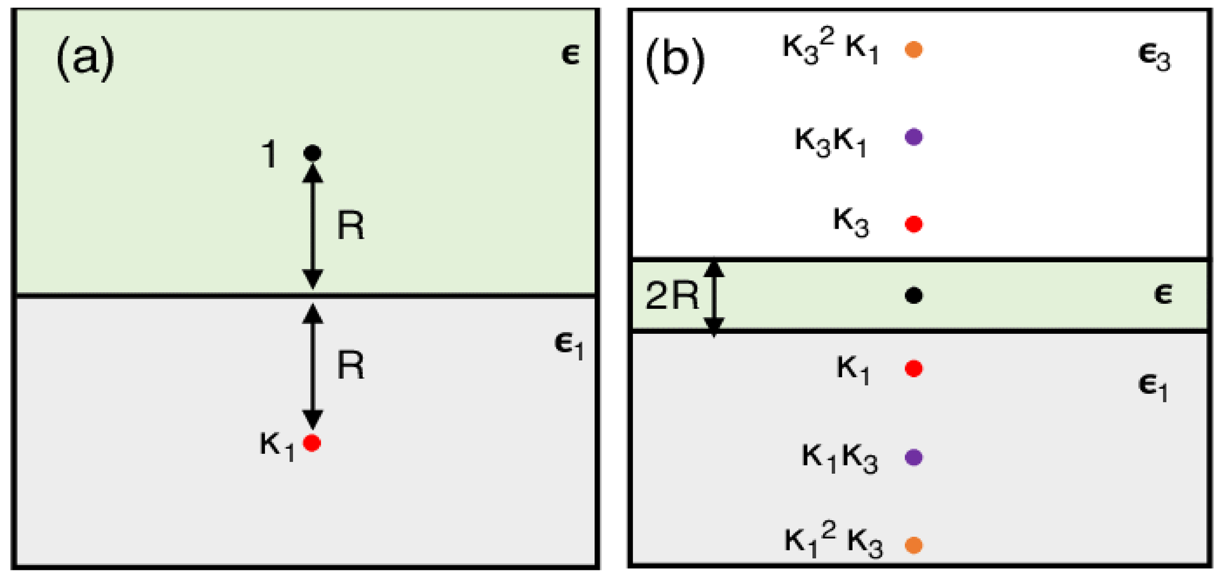
https://advanced.onlinelibrary.wiley.com/doi/10.1002/adom.202102698



https://www.researchgate.net/figure/Exciton-levels-for-a-simple-band-structure-at-0-k

Muljarov Superlattice Analysis

- When a charged particle (electron) is placed near another material with a different dielectric constant an image charge is formed.
- When you have layered materials, image charges create new image charges.
- These image charges create a slight difference in the potential V(ρ).
- The potential V(ρ) is used to solve the Schrodinger equation.
- Each perovskite will have a different potential, thus different electronic properties.



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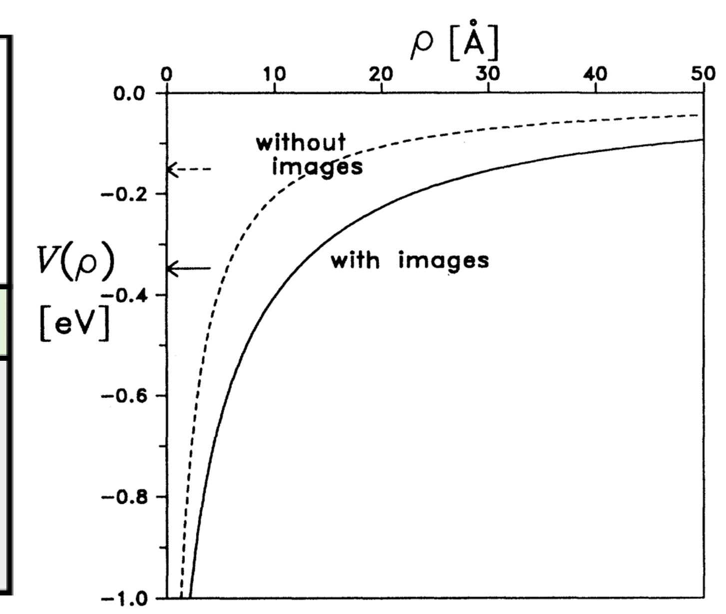
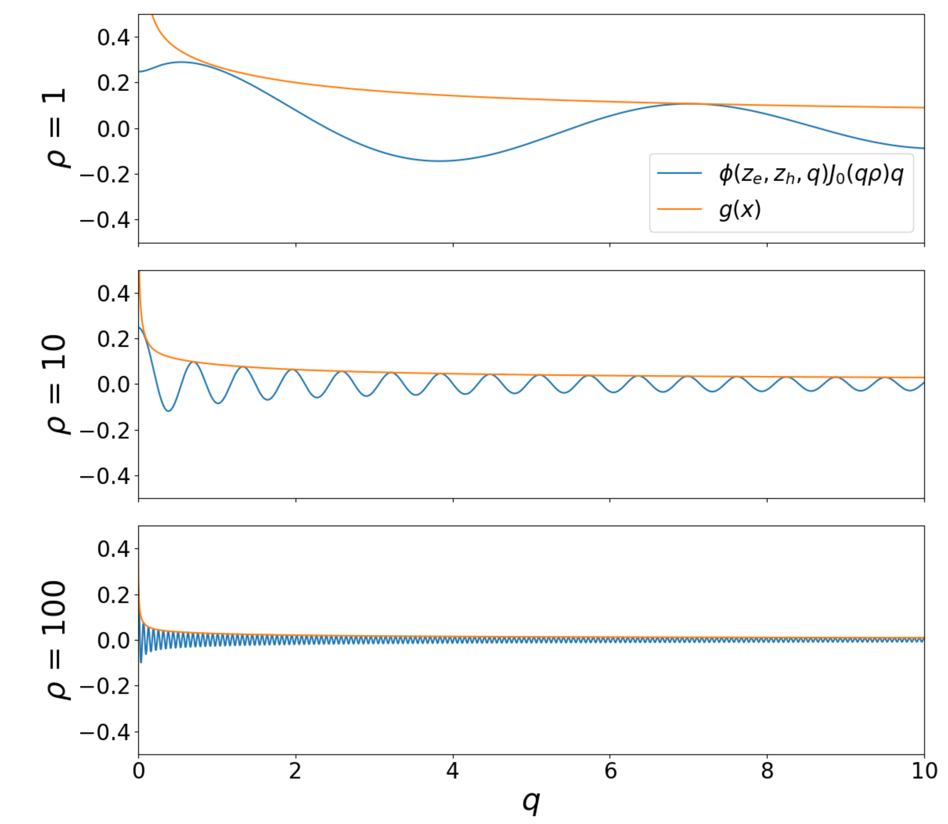


Muljarov, Egor A., et al. Physical Review B 51.20 (1995): 14370

Integral Formula

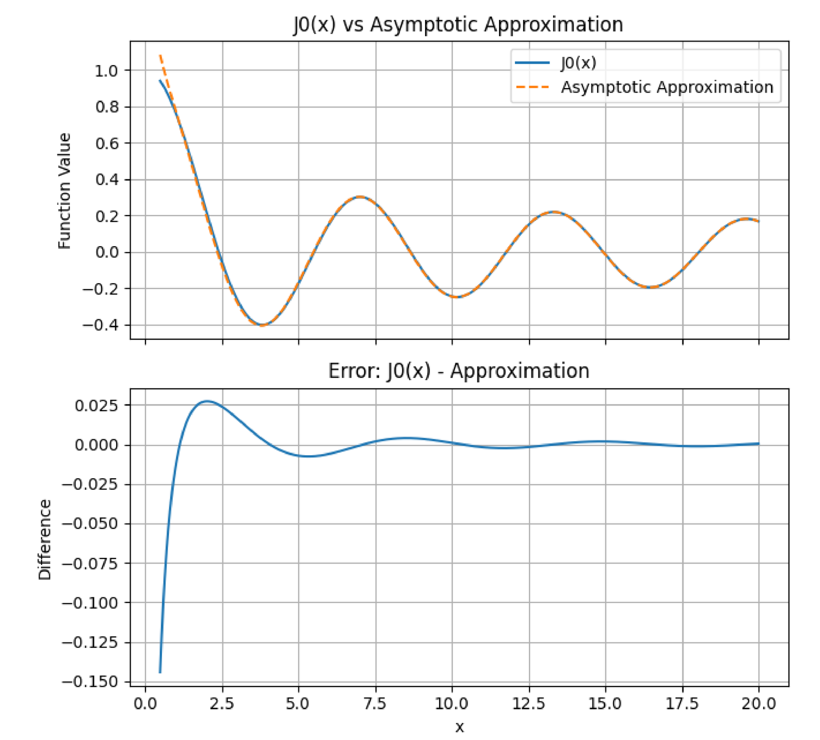


- To solve the potential V(ρ) we must integrate 1000's of times at each ρ.
- Filon integration works for every value of ρ without an increase in computation time.

$$\int_0^\infty \frac{e}{2\pi}\,\phi_{A78}(z_e, z_h, q, v)\, J_0(q\,\rho)\, q\, dq$$

$$J_0(x) \approx \sqrt{\frac{2}{\pi x}}\cos(x - \pi/4) + O_2(x)$$

Approximation



Filon Integration

- Filon Integration is an integration technique that integrates a function f(x) with an oscillatory term.

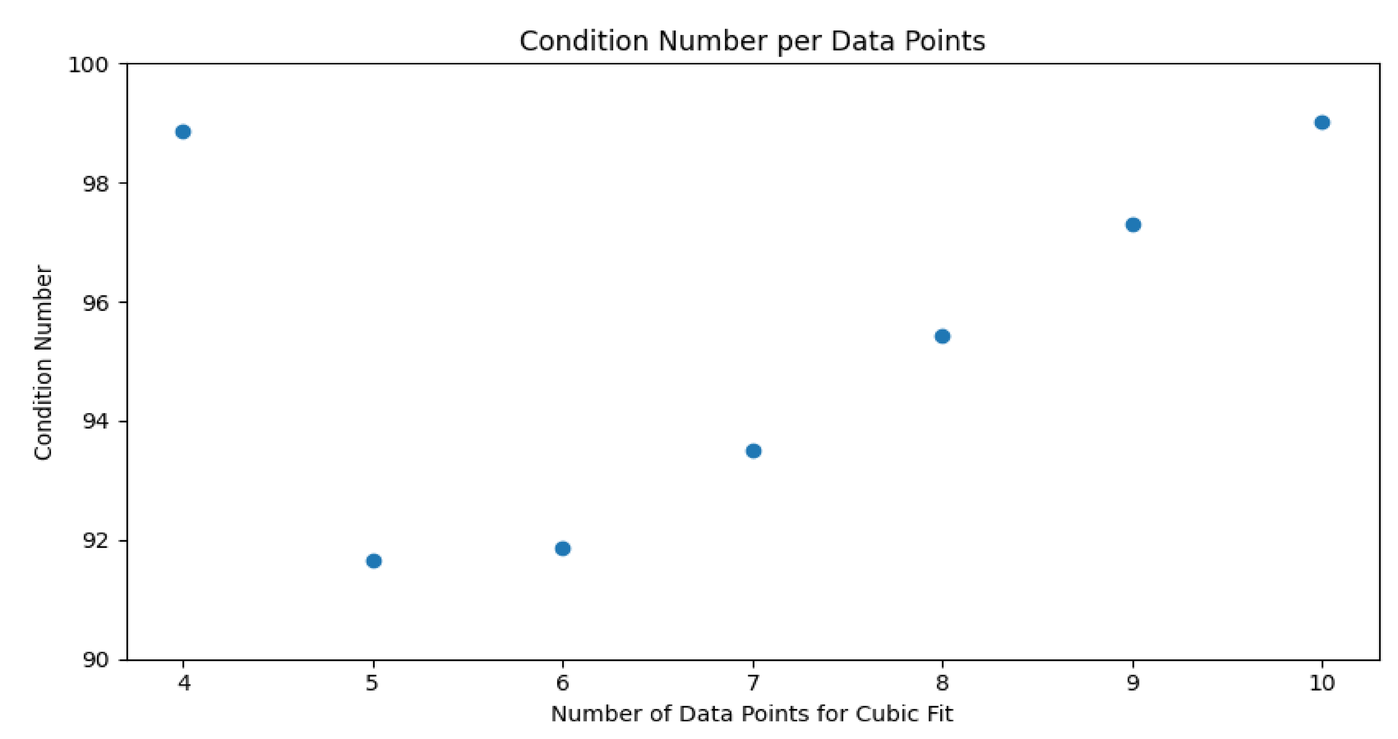
$$I = \int_a^b f(x)\, e^{i\omega x}\, dx, \rightarrow A\int_a^b f(x)\; g(\omega x)\, dx,$$

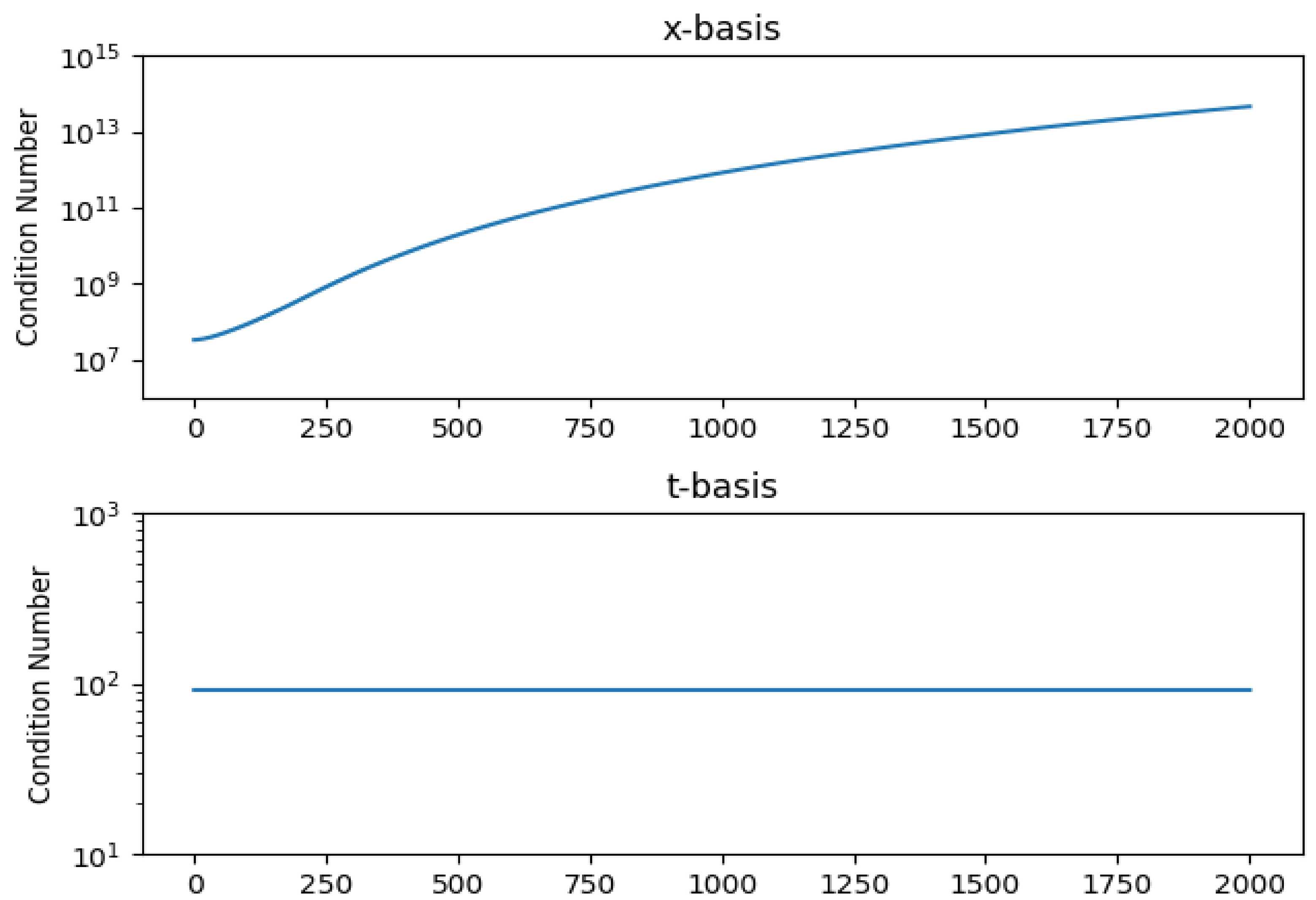
- To make this work we can separate our integrand:

$$f(\mathrm{x}) = \mathrm{x}\,\phi_{A78}(z_e, z_h, \mathrm{x}, \mathrm{v}), \qquad g(\omega \mathrm{x}) = J_0(\omega \mathrm{x})$$

- The above equations can be approximated as a cubic function and a sinusoidal function.

$$f(x) = a + bx + cx^2 + dx^3, \qquad g(\omega x) = \cos(x - \pi/4)$$





- In the x-basis the polynomial fit has data points are very close to each other and become very large when cubed.
- In the t-basis the fits are performed between 0 and 1 keeping the cubic term always less than 1.
- In the t-basis the figure to the left shows that 5 data points gives the best results without overfitting.

Conclusions/Future Research

- Changing bases gives the same result, increases stability of the solution, and decreases catastrophic cancelation likelihood.
- Filon integration allows calculates the integral with only a 0.2% percent error with jax optimization and speed.
- In the future more analysis can be done to see if the original integral could be solved in the qρ basis instead of just the q basis. This would decrease the computational load on the computer and decrease computational time exponentially.
- Git Repository: https://github.com/MrPhysics1/Physics580