Background material

Fermions: Particles (e.g. electrons) with certain traits

- Wavefunction antisymmetric for particle exchange
- Pauli exclusion principle
- Boltzmann distribution for noninteracting: $Q = \prod_k \left(1 + e^{-\beta(\epsilon_k - \mu_k)}\right)$

Second quantization: "Ladder operator" description of QM

- Everything is quantized; state defined by quanta
- Use occupation numbers as basis $|\mathbf{n}\rangle = |n_1, n_2, \ldots\rangle$
- Creation operator $\hat{a}_i^\dagger |\mathbf{0}\rangle = |n_1 = 0, \ldots, n_i = 1, n_{i+1} = 0, \ldots\rangle$
- Annihilation operator $\hat{a}_i |\mathbf{1}\rangle = |n_1 = 1, \ldots, n_i = 0, n_{i+1} = 1, \ldots\rangle$

Why create another approach for molecular electronics?

Molecular Electronics

Second quantization

Vibrational Motion

Classical potentials

These are two different languages.
We need to translate from one to the other.