# Machine Learning in Quantum Mechanics

**Normalizing Flows for Computing Molecular Vibrational Wave Functions** 

Nicolas Mendoza Hamburg, 07.09.2022



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# Introduction



Solving Schrödinger's Equation is hard

$$E_{t,ij} = \sum_{k,l} \sum_{\lambda_i,\lambda'_i} \rho_{\lambda_1,\lambda'_1}(e_1^-) \rho_{\lambda_2,\lambda'_2}(e_2^-) [T_{ij}^{\lambda_1 \lambda_2}(\tilde{\chi}_k^0)] \cdot [T_{ij}^{\lambda'_1 \lambda'_2}(\tilde{\chi}_k^0)]^*$$

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- Solving Schrödinger's Equation is hard
- > Usually turn to numerical approximations

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- ...but numerics have limitations

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- Solving Schrödinger's Equation is hard
- > Usually turn to numerical approximations
- ...but numerics have limitations
- > The Curse of Dimensionality

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#### Thank you!

#### Contact

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