Studies of Quantum Dots using Machine Learning

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Outline

Quantum mechanics

Machine learning

Our approach

Results

Quantum Mechanics

$$i\hbar \frac{\partial}{\partial t} |\Psi(\boldsymbol{r}, t)\rangle = \hat{\mathcal{H}} |\Psi(\boldsymbol{r}, t)\rangle$$

The time-independent Schrödinger equation

$$E_n = \frac{\int d\boldsymbol{r}\Psi_n^*(\boldsymbol{r})\hat{\mathcal{H}}\Psi_n(\boldsymbol{r})}{\int d\boldsymbol{r}\Psi_n^*(\boldsymbol{r})\Psi_n(\boldsymbol{r})}$$

Harmonic oscillator

$$\hat{\mathcal{H}} = \sum_{i=1}^{N} \left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2 \right)$$

Quantum dots

Many-body problem

$$\hat{\mathcal{H}} = \sum_{i=1}^{N} \left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2 \right) + \sum_{i<j} \frac{1}{r_{ij}}$$

Variational Monte Carlo

$$
\begin{aligned}
E_0 < E &= \frac{\int d\boldsymbol{r}\Psi_0(\boldsymbol{r})^* \hat{\mathcal{H}} \Psi_0(\boldsymbol{r})}{\int d\boldsymbol{r}\Psi_0(\boldsymbol{r})^* \Psi_0(\boldsymbol{r})} \\
&= \int d\boldsymbol{r} E_L(\boldsymbol{r}) P(\boldsymbol{r}) \\
&\approx \frac{1}{M} \sum_{i=1}^{M} E_L(\boldsymbol{r}_i)
\end{aligned}
$$

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Slide 7

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Slide 8

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Slide 9

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Slide 10

something, something something

Slide 11

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Slide 12

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Slide 13

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Slide 14

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Slide 15

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Slide 16

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