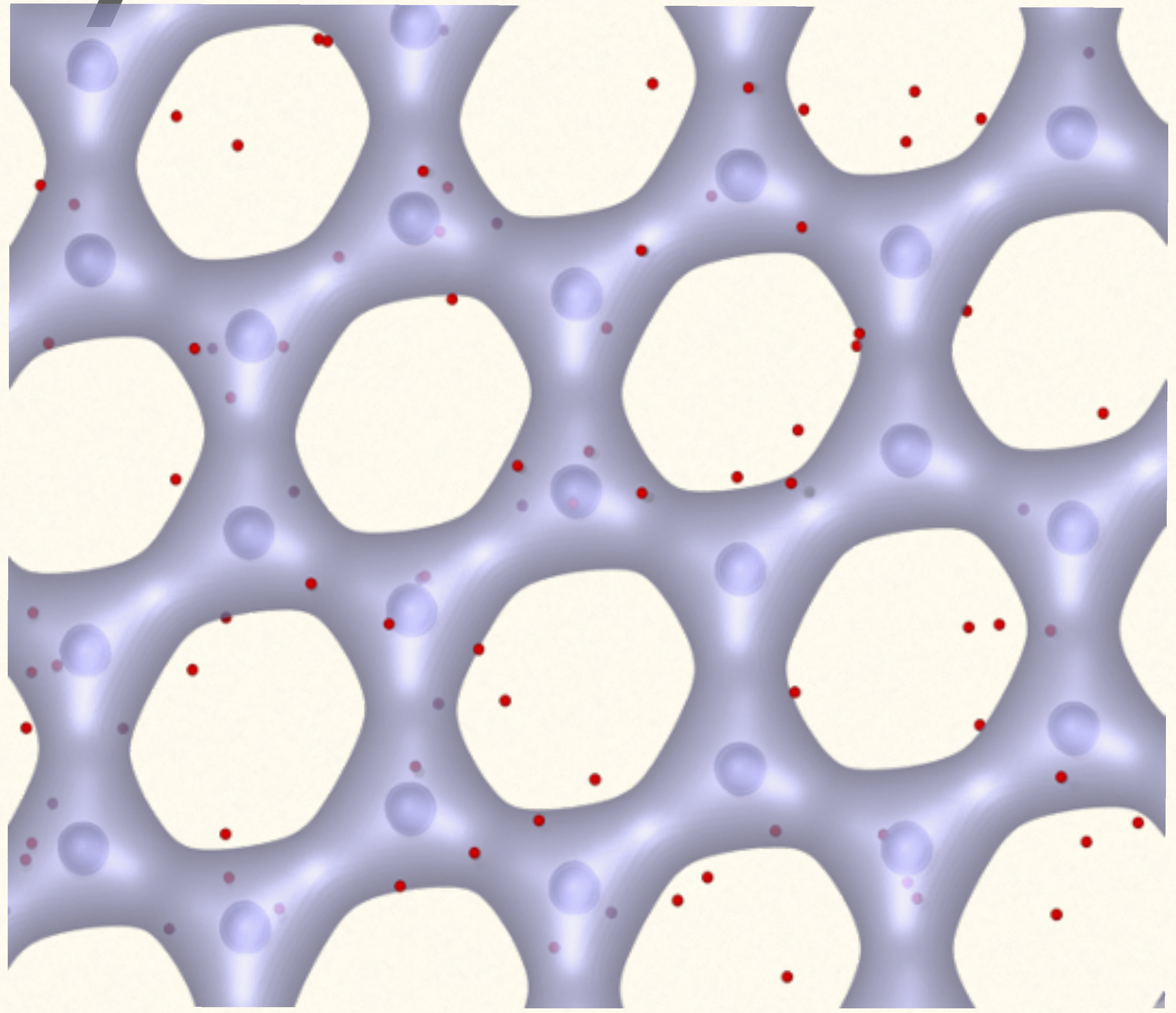
# Introduction to computational physics and computing $\pi$

PHYS 246 class 1

https://lkwagner.github.io/IntroductionToComputationalPhysics/intro.html

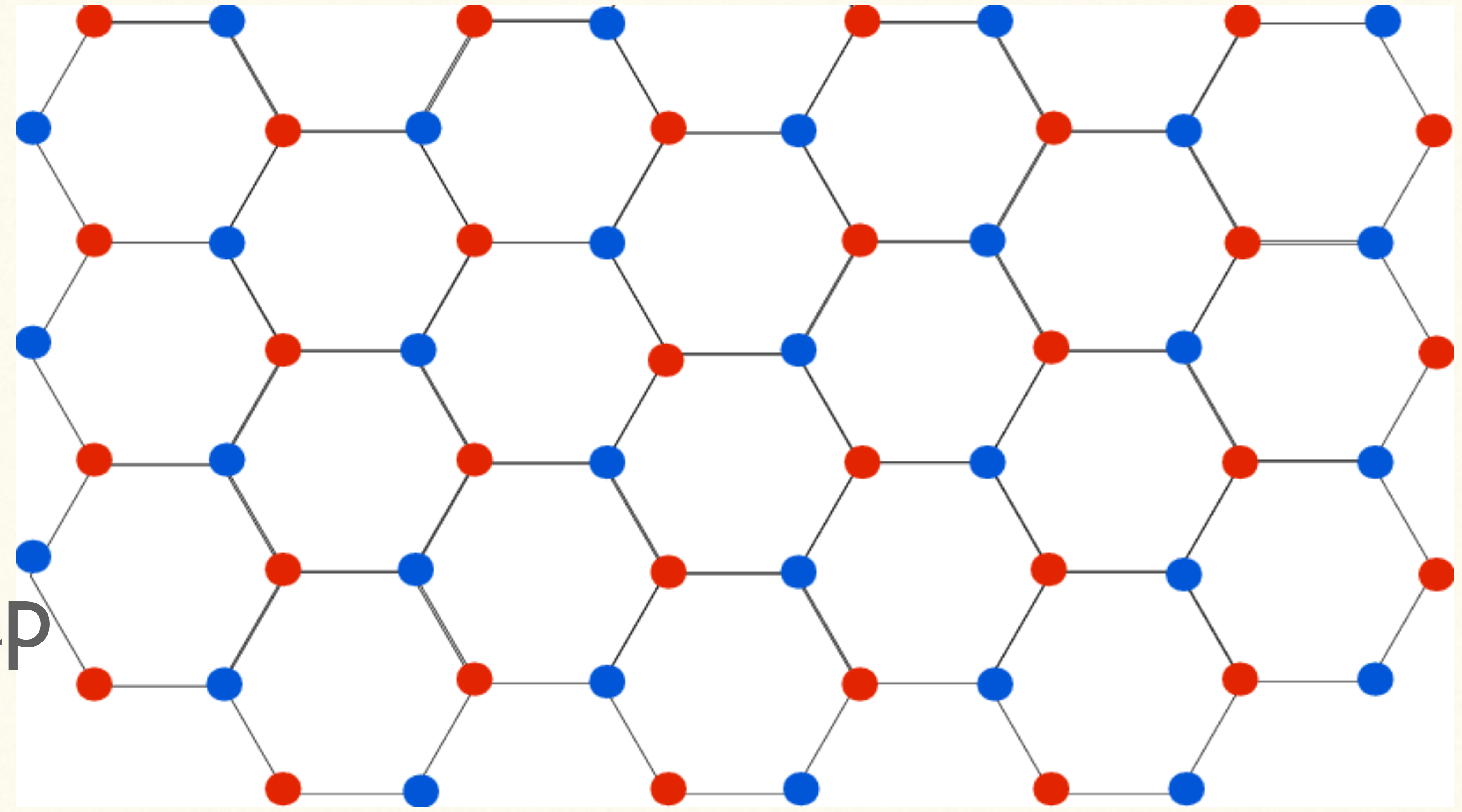
# My research



$$\hat{H} = -\sum_i \frac{\nabla_i^2}{2} - \sum_{i\alpha} \frac{Z_\alpha}{r_{i\alpha}} + \sum_{ij} \frac{1}{r_{ij}} + \ldots$$

First principles calculations: universal physics for all condensed matter systems.

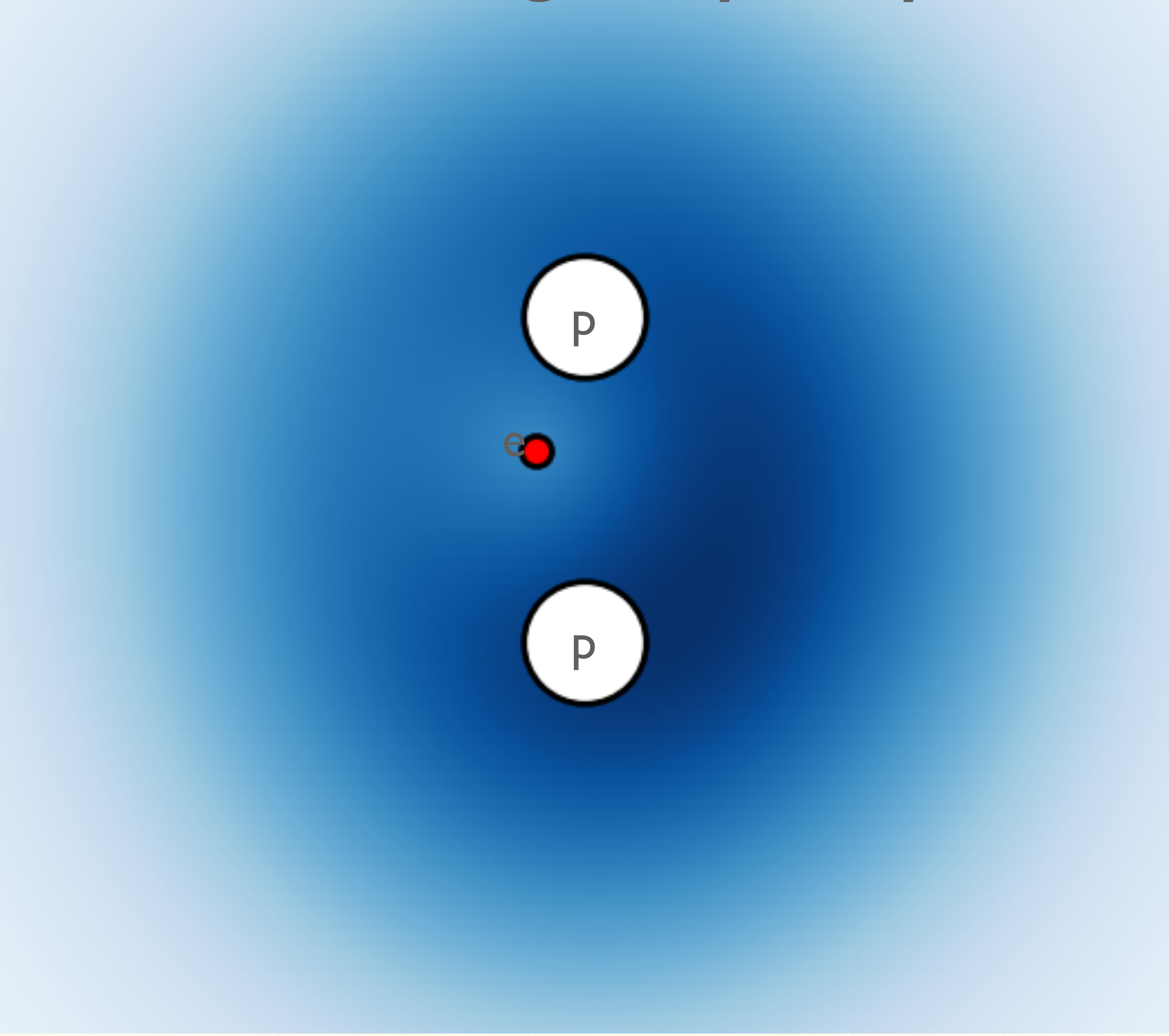
Data to bridge the gap



$$\hat{H} = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$

Effective models: specific, simpler models for a particular material

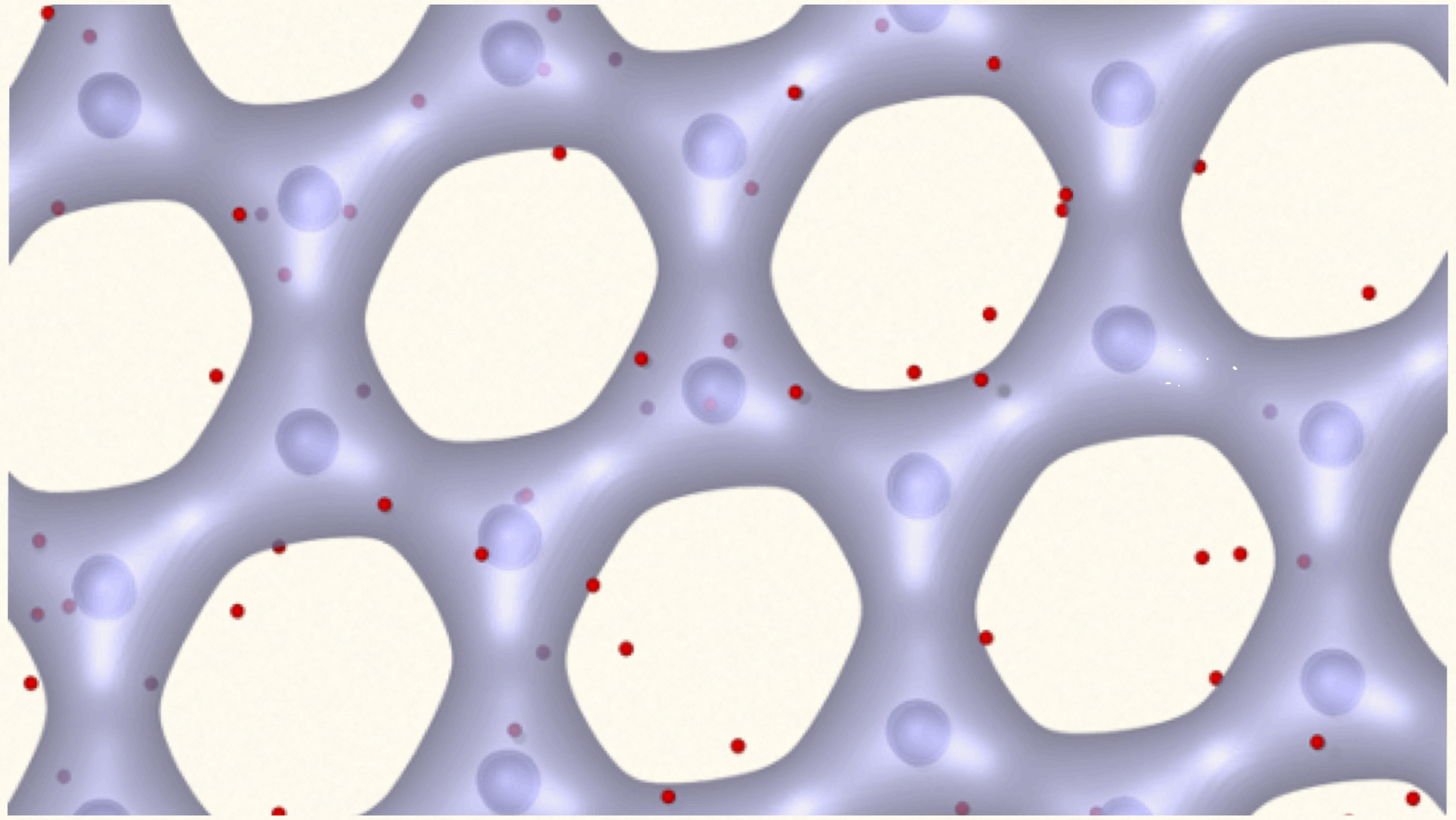
# Understanding many-body wave functions: weak correlation




Two electron and two protons

Conditional wave function:
$\Psi(x_1 \,|\, x_2, r_1, r_2)$

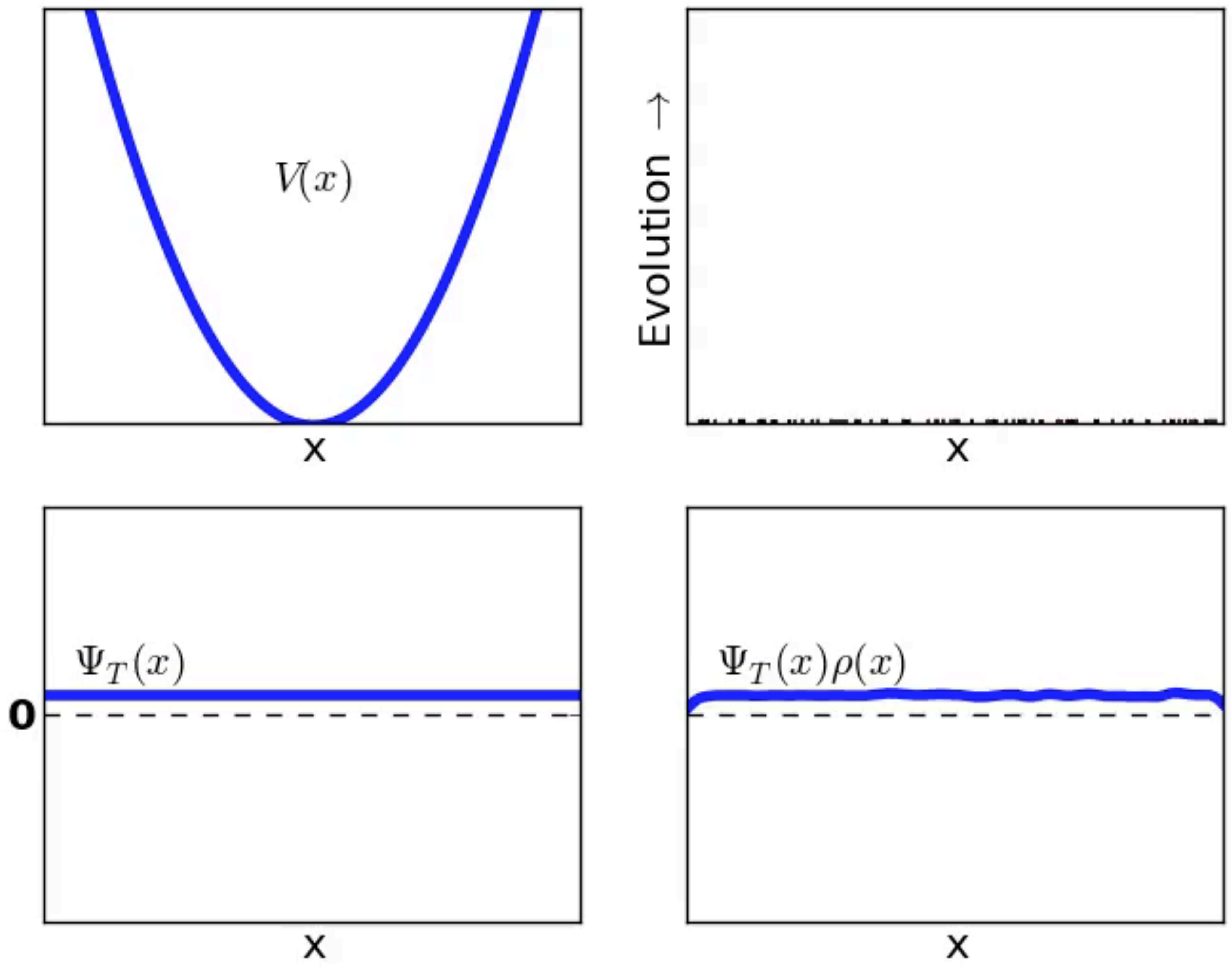
# Efficient description of correlation using Monte Carlo



Represent the wave function as a sum of "walkers"

$$\Psi(x) = \sum_i w_i \delta(x - x_i)$$

Weights and positions determined by a stochastic process.

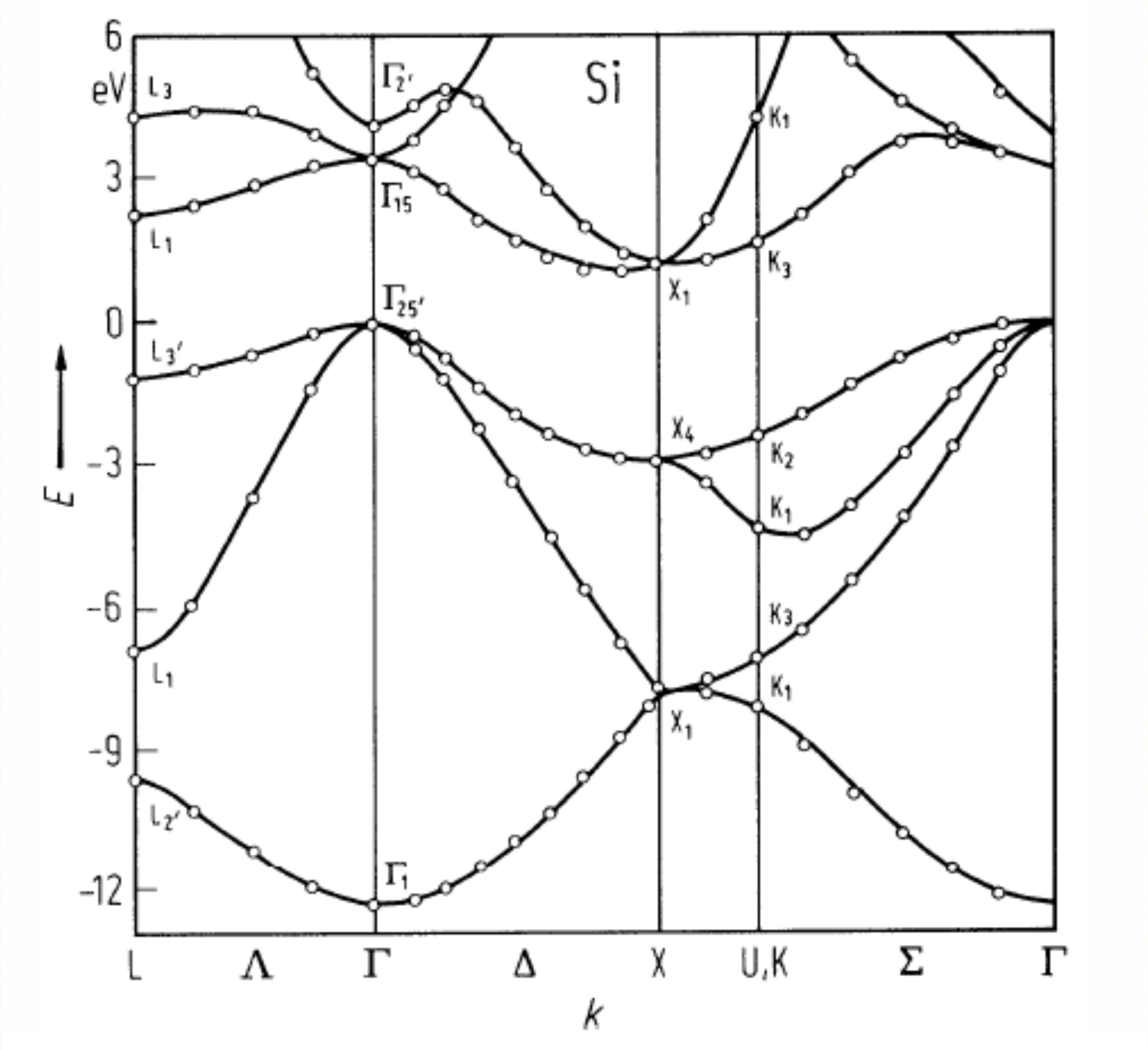


# Weak correlation is strong but can be coarse-grained out

Silicon

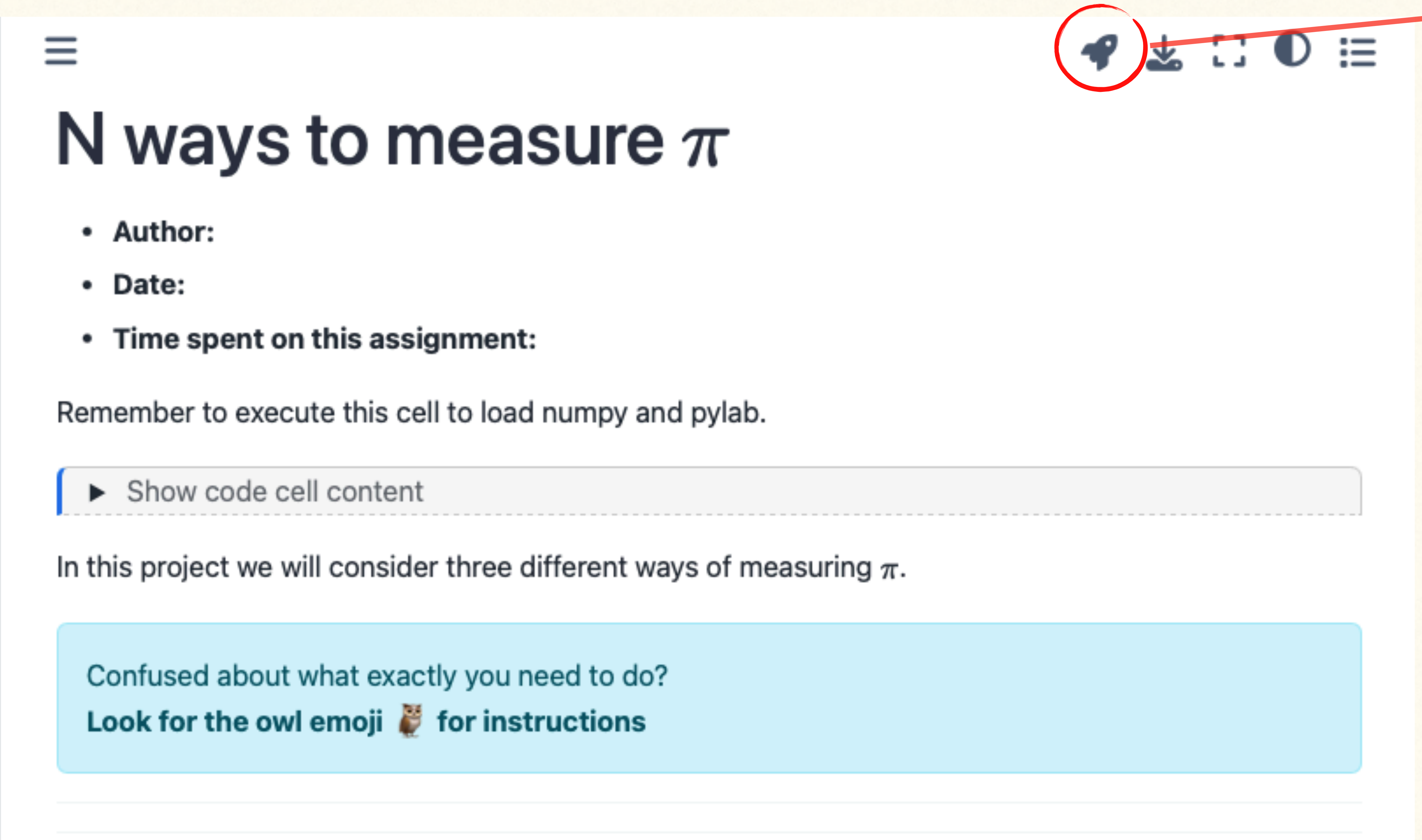
Band gap ignoring electron correlations: 5 eV

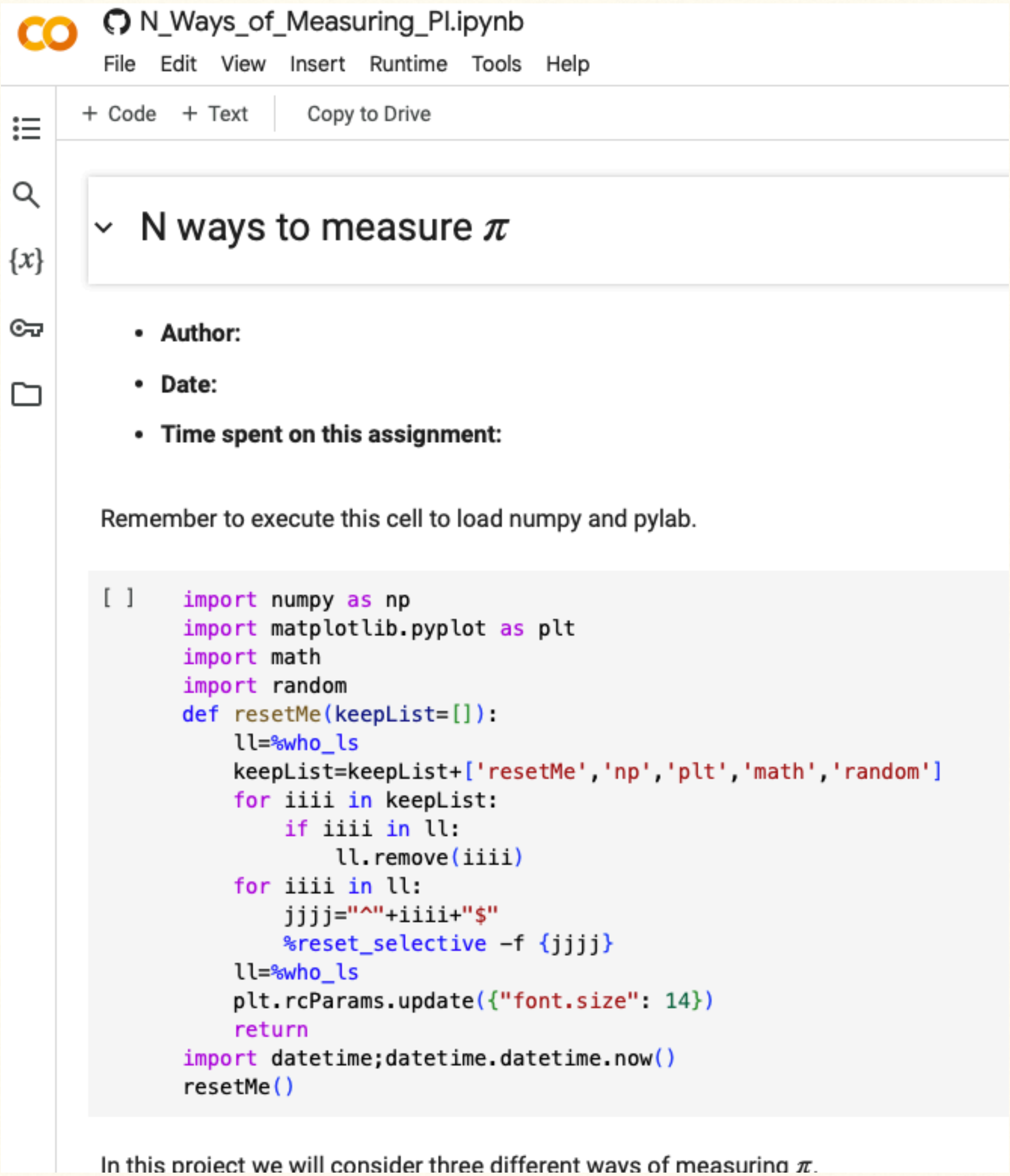
Band gap in reality: 1.1 eV




Source: O. Madelung, U. Rössler, M. Schulz (ed.) SpringerMaterials Silicon (Si), band structure Landolt-Börnstein - Group III Condensed Matter 41A1b (Group IV Elements, IV-IV and III-V Compounds. Part b - Electronic, Transport, Optical and Other Properties) http://materials.springer.com/lb/docs/sm_lbs_978-3-540-31356-4_432 10.1007/10832182_432 (Springer-Verlag Berlin Heidelberg ©2002) Accessed: 14-01-2016

# Getting started



# Python notebooks

Runtime environment

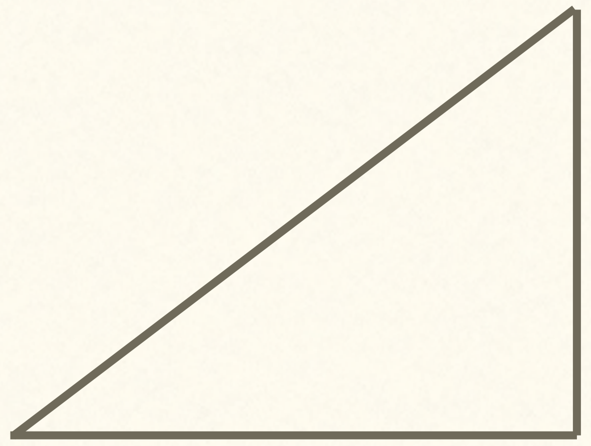
```
[1]    x = 5

[2]    x = 6

[3]    print(x)

       6
```

```
0s  [2]    x = 5

0s  [1]    x = 6

0s  [3]    print(x)

           5
```

# Submitting your work

- Work is due one week after the class.
- You should be added to the canvas class.
- Upload a PDF (I'll send out detailed instructions over the email)
- Share your colab instance with us
- Remember to not change your colab instance once you submit your work!

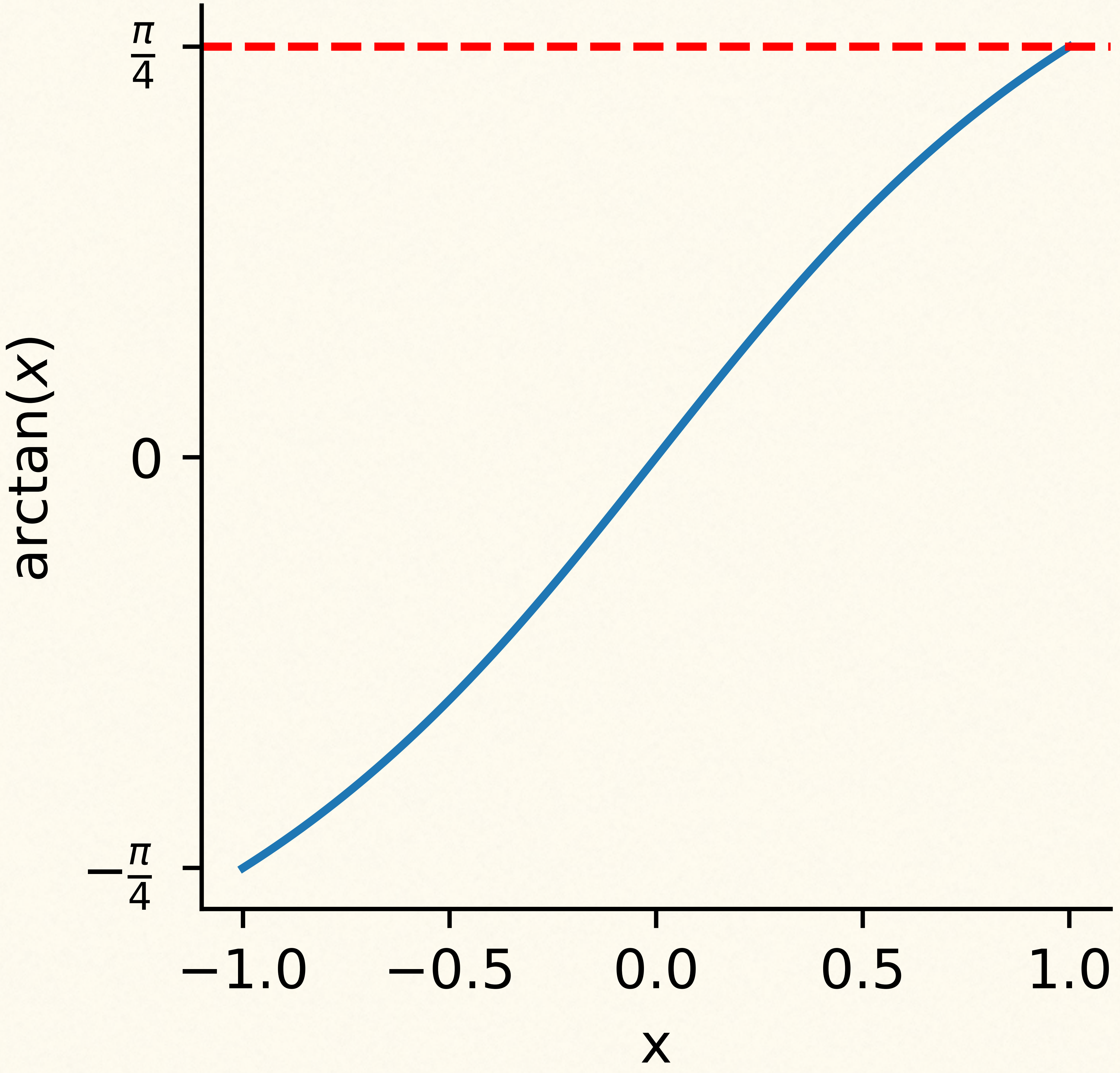
# Methods to compute $\pi$



Note that $\arctan(1) = \pi/4$

Expand in a Taylor series around 0:

$$\tan^{-1}(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} x^{2n+1}; -1 < x \leq 1$$



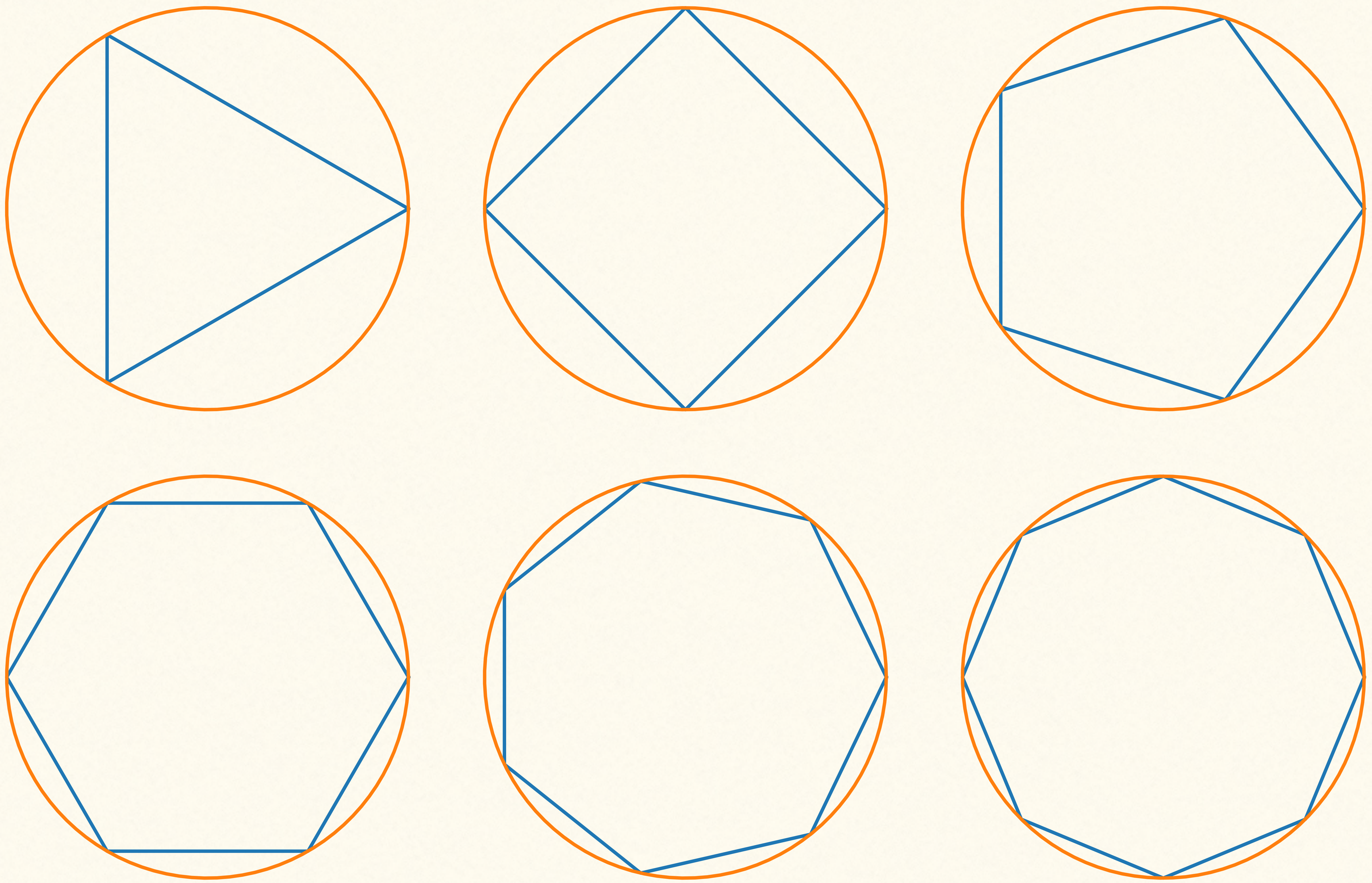
# Ramanujan

$$\frac{1}{\pi} = \frac{2\sqrt{2}}{9801} \sum_{k=0}^{\infty} \frac{(4k)!(1103 + 26390k)}{(k!)^4 396^{4k}}$$

Surprisingly difficult to show!

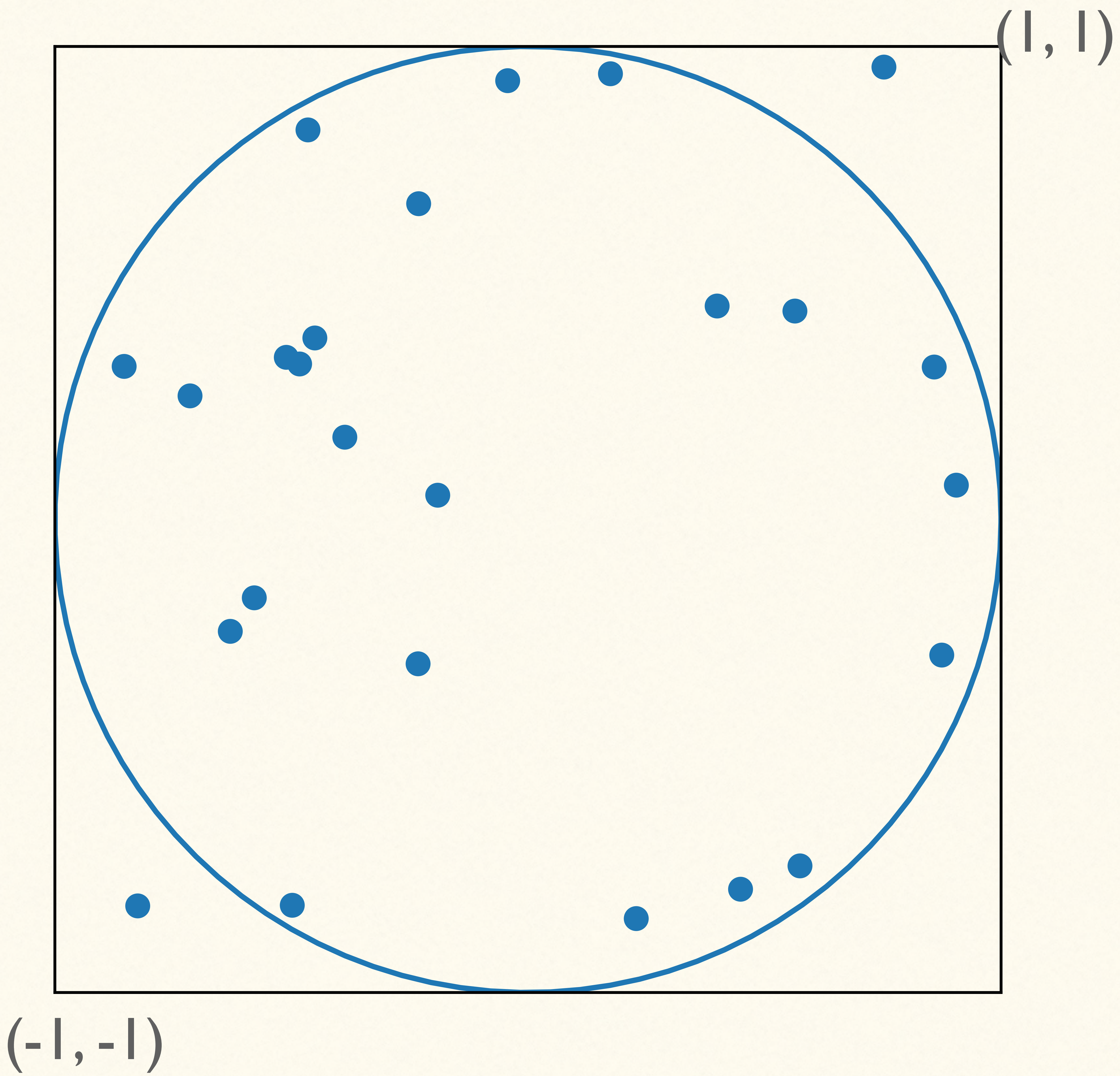
Detailed explanation here:
https://paramanands.blogspot.com/2012/03/modular-equations-and-approximations-to-pi-part-1.html?m=0

# Archimedes



The circumference of a polygon of degree N approaches that of a circle as $N \to \infty$.

# Monte Carlo (random numbers)




Area of the circle: $\pi$
Area of the square: 4

Proportion of random throws that land within the circle: $\pi/4$

# Averaging and uncertainty

Consider a random variable $x$ with expectation value $\langle x \rangle$ and standard deviation $\sigma$.

Construct a random variable $x_n = \dfrac{1}{n}\sum_{i=1}^{n} x_i$ as the average of $n$ samples of $x$.

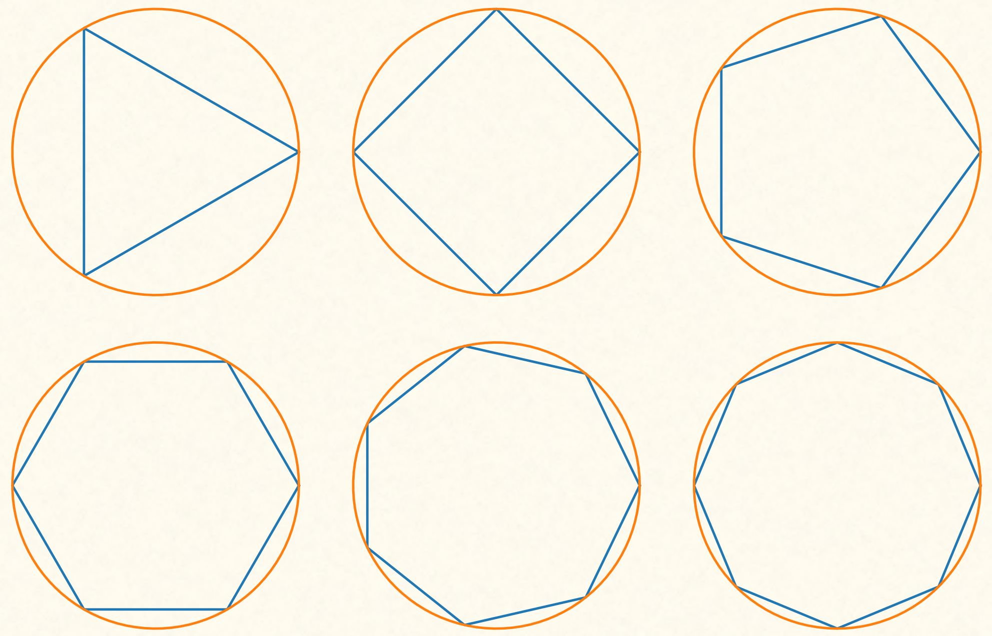
Central limit theorem:
$x_n \sim N(\langle x \rangle, \sigma_n)$, where $\sigma_n = \dfrac{\sigma}{\sqrt{n}}$

# Discussion question

We saw ~four methods to compute $\pi$.

What do you think the pluses and minuses might be for these methods?

How to evaluate them against one another?



$$\arctan(1) = \pi/4$$

$$\frac{1}{\pi} = \frac{2\sqrt{2}}{9801}\sum_{k=0}^{\infty}\frac{(4k)!(1103 + 26390k)}{(k!)^4 396^{4k}}$$