Computational Quantum Physics
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1 Introduction

Computational physics generally concerns the solution of physics problems with the help of a computer. Such a problem can be the evaluation of a concrete property of the model, such as a scattering cross section or a susceptibility, to which no analytical solution exists. Often, however, the models considered are too complicated to even formulate such quantities. Then, the whole system (dynamics) is simulated, similar to an actual experiment. Due to this dichotomy, computational physics is often considered a third pillar of physics research, see Fig. 1.

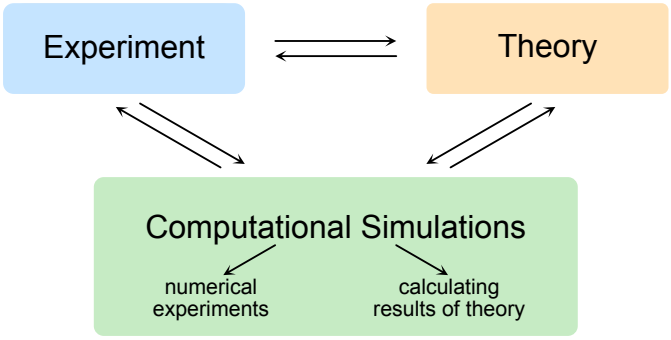


Figure 1: Role of computational simulations in modern physics.

When dealing with quantum mechanical problems—the subject of this course—problems emerge not encountered in classical mechanics. While in the latter, a collection of particles lives in the phase space, a quantum mechanical state is an element of an (exponentially) larger Hilbert space. In order to make progress, we thus need to decide what "kind of solution" we are interested in. For a single particle, we might be able to calculate the wave function or a scattering cross section exactly. For an interacting many particle system, only approximate solutions are available, which vary depending on the properties of the system we are interested in. Figure 2 provides an overview over the various approaches and their organization within this course.

While the development of new methods and algorithms in computational quantum physics is an active field, the aim of this course is for students to understand the basic concepts and master the necessary tools for their own applications. Thus, after this course

- students are able to describe the difficulties of quantum-mechanical simulations,
- students are able to explain the strengths and weaknesses of the methods covered,
- students are able to select an appropriate method for a given problem,
- students are able to implement basic versions of all algorithms discussed.

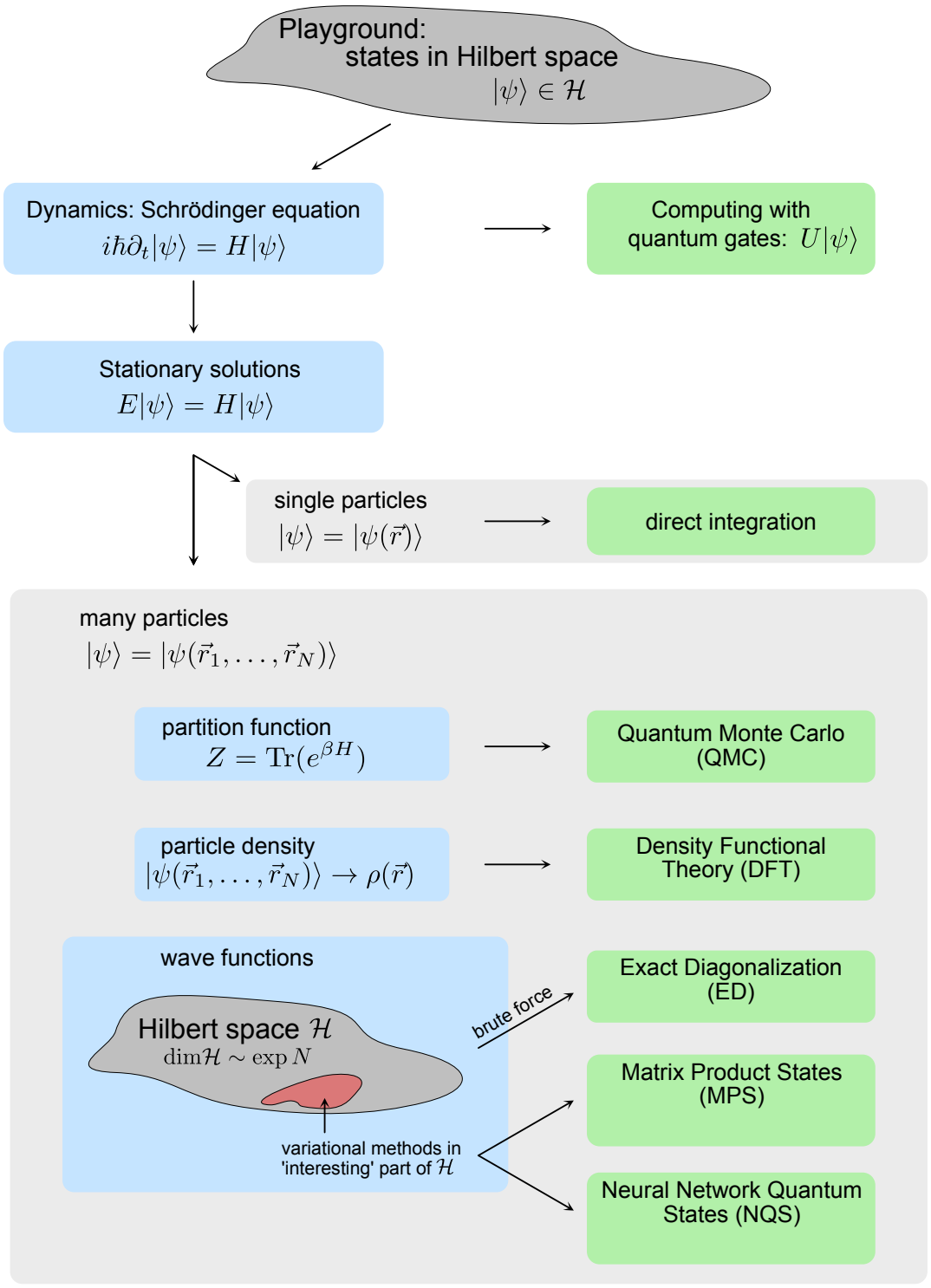


Figure 2: Overview of challenges and methods of computational quantum physics.

1.1 Prerequisites and tools

For this course, we assume the following prerequisites:

- While we will introduce the main concepts of quantum mechanics at the beginning of the semester to refresh your knowledge, a basic knowledge is assumed.
- Basic knowledge of numerical tools, such as numerical differentiation and integration, linear solvers, eigensolvers, root solvers, optimization.
- Basic knowledge of a programming language. For the teaching assignments, you are free to choose your preferable one. The solutions will typically be distributed in Python in the form of Jupyter notebooks.

Please, don't hesitate to ask questions if any notions are unclear.

1.2 References

For further reading, we recommend the following books and reviews:

- **General:** *Computational Physics*, Jos Thiisen (Cambridge University Press)
- **ED:** *Computational Studies of Quantum Spin Systems*, A. W. Sandwik, AIP Conference Proceedings **1297**, 135 (2010)
- **DMRG:** *The density-matrix renormalization group in the age of matrix product states*, U. Schollwöck, Annals of Physics **326**, 96 (2011)
- **Monte Carlo:** *Quantum Monte Carlo Approaches for Correlated Systems*, F. Becca and S. Sorella (Cambridge University Press)
- **DFT:** *Electronic Structure, Basic Theory and Practical Methods*, R. M. Martin (Cambridge University Press)

Note that publications by Cambridge University Press are available as online resources within the ETHZ network (including eduroam).

2 Quantum mechanics crash course

The following pages cannot replace a proper introduction to quantum mechanics. However, they serve as a refresher and should fix our notation.

2.1 The basics

2.1.1 Wave functions and the Hilbert space

Quantum mechanics is in essence linear algebra. The ingredients are simple: A pure state of a quantum system is described by a wave function, which is an element of a Hilbert space

$$|\psi\rangle \in \mathcal{H}. \tag{2.1}$$

As the wave function has the interpretation of a probability distribution, we typically work with normalized wave functions

$$\||\psi\rangle\| \equiv \sqrt{\langle\psi|\psi\rangle} = 1. \tag{2.2}$$

Here and in the following, we use the bra-ket notation and $\langle\psi|\varphi\rangle$ is the scalar product of two elements $|\psi\rangle$ and $|\varphi\rangle$ in $\mathcal{H}$.

The canonical example of a simple Hilbert space is a spin-1/2 system, for example the two spin states of an electron. Classically, the spin $\vec{S}$ of an electron can point in any direction. In quantum mechanics, this is encoded in the complex two-dimensional Hilbert space $\mathcal{H} = \mathbb{C}^2$. Usually, we use the basis states

$$\text{"up"}: |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad \text{"down"}: |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

This is reminiscent of the Ising model, though here, the spin state can be in any superposition

$$|\psi\rangle = \alpha\,|\uparrow\rangle + \beta\,|\downarrow\rangle \tag{2.3}$$

with $|\alpha|^2 + |\beta|^2 = 1$. In particular,

$$|\rightarrow\rangle = \frac{1}{\sqrt{2}}\big(\,|\uparrow\rangle + |\downarrow\rangle\,\big) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{2.4}$$

is oriented in the positive x-direction.

2.1.2 Observables and Operators

Any physical observable is represented by a self-adjoint linear operator acting on $\mathcal{H}$. For a finite-dimensional $\mathcal{H}$, this means the observable can be represented by a hermitian matrix.

For the spin-1/2 example, the components of the angular momentum are represented by

$$\begin{aligned}\hat{S}^x &= \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\\ \hat{S}^y &= \frac{\hbar}{2}\sigma_y = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\\ \hat{S}^z &= \frac{\hbar}{2}\sigma_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\end{aligned} \tag{2.5}$$

where σ_x, σ_y, σ_z are the Pauli matrices. For a spin pointing along an arbitrary direction $\hat{\mathbf{e}} = (e_x, e_y, e_z)$, we write

$$\hat{\mathbf{e}} \cdot \hat{\vec{S}} = \frac{\hbar}{2}\begin{pmatrix}e_z & e_x - ie_y\\ e_x + ie_y & -e_z\end{pmatrix}. \tag{2.6}$$

Note that

$$\begin{aligned}[\hat{S}^x, \hat{S}^y] &\equiv \hat{S}^x\hat{S}^y - \hat{S}^y\hat{S}^x = i\hbar\hat{S}^z,\\ [\hat{S}^y, \hat{S}^z] &= i\hbar\hat{S}^x,\\ [\hat{S}^z, \hat{S}^x] &= i\hbar\hat{S}^y.\end{aligned} \tag{2.7}$$

The spin operators don't commute.

2.1.3 Schrödinger equation

The equation governing the dynamics of a quantum state is the Schrödinger equation

$$i\hbar\partial_t \left|\psi\left(t\right)\right\rangle = \hat{H}\left|\psi\left(t\right)\right\rangle, \tag{2.8}$$

where $\hat{H}$ is the Hamilton operator, or Hamiltonian, encoding the energy of the system. Equation (2.8) is a *first-order* linear differential equation.

For a stationary solution of the Schrödinger equation we can use the ansatz

$$\left|\psi\left(t\right)\right\rangle = e^{-iEt/\hbar}\left|\psi\left(0\right)\right\rangle, \tag{2.9}$$

where E is the energy of the system. The Schrödinger equation then simplifies to a linear eigenvalue problem

$$\hat{H}\left|\psi\right\rangle = E\left|\psi\right\rangle. \tag{2.10}$$

2.1.4 Mixed states and density matrix

Unless perfectly isolated, a system is not in a pure state $|\psi\rangle$, but rather in an incoherent mixture of several states. Such a general state is described by a density matrix ρ, a positive semidefinite *operator* with

$$\mathrm{Tr}(\rho) = 1. \tag{2.11}$$

For a pure state $|\psi\rangle$, the density matrix is given by

$$\rho_{\mathrm{pure}} = \left|\psi\right\rangle\left\langle\psi\right|. \tag{2.12}$$

For the example of a spin pointing in the x-direction, we find

$$\rho_{\rightarrow} = |\rightarrow\rangle\langle\rightarrow| = \frac{1}{2}\begin{pmatrix}1\\1\end{pmatrix}\begin{pmatrix}1 & 1\end{pmatrix} = \begin{pmatrix}1/2 & 1/2\\1/2 & 1/2\end{pmatrix}. \tag{2.13}$$

More generally, we can write a density matrix as

$$\rho = \sum_{i,j} p_{ij} |\psi_i\rangle\langle\psi_j| . \tag{2.14}$$

For example, for a system in a probabilistic mixture of the pure states $|\uparrow\rangle$ and $|\downarrow\rangle$, the density matrix reads

$$\rho_{\text{mixed}} = \begin{pmatrix}1/2 & 0\\0 & 1/2\end{pmatrix}. \tag{2.15}$$

Finally, we define the purity of the system as $\mathrm{Tr}\left(\rho^2\right)$ [Compare $\mathrm{Tr}\left(\rho^2_{\text{pure}}\right)$ and $\mathrm{Tr}\left(\rho^2_{\text{mixed}}\right)$].

The unitary time evolution of the density matrix follows from Eqs. (2.14) and (2.8) as

$$i\hbar\partial_t\rho(t) = \left[\hat{H}, \rho(t)\right]. \tag{2.16}$$

2.1.5 Thermal density matrix

Often, we want to describe a physical system, which is not in its ground state, but in thermal equilibrium at a given temperature T (inverse temperature $\beta = 1/k_B T$). In a classical system, each state i of energy E_i is occupied with a probability given by the Boltzmann distribution

$$p_i = \frac{1}{Z} e^{-\beta E_i} \tag{2.17}$$

with $Z = \sum_i e^{-\beta E_i}$ the partition function. We have already seen how to describe statistical mixtures through the density matrix: In a quantum system, knowing the basis of eigenstates $|i\rangle$ with energy E_i,

$$\hat{H}|i\rangle = E_i|i\rangle , \tag{2.18}$$

the thermal density matrix can be written analogously as

$$\rho_\beta = \frac{1}{Z}\sum_i e^{-\beta E_i} |i\rangle\langle i| . \tag{2.19}$$

Unfortunately, we usually don't know $|i\rangle$, as this requires full diagonalization of the Hamiltonian. In general, the density matrix can be written as

$$\rho_\beta = \frac{1}{Z} e^{-\beta\hat{H}} \tag{2.20}$$

with

$$Z = \mathrm{Tr}\left(e^{-\beta\hat{H}}\right). \tag{2.21}$$

2.1.6 Measurement process

A measurement in a quantum system is (usually) intrusive and the outcome is not deterministic. After measuring an observable A, the wave function of the system collapses to an eigenvector of $\hat{A}$ and the outcome of the measurement is given by the respective eigenvalue. The state of the system is thus changed by the measurement process.

Typically, we are not interested in a single measurement, but in the average value of an operator $\hat{A}$. This expectation value can be calculated in the general case as

$$\langle \hat{A} \rangle = \mathrm{Tr}\Big(\rho \hat{A}\Big). \tag{2.22}$$

For a pure state $\rho = |\psi\rangle \langle\psi|$, Eq. (2.22) reduces to

$$\langle \hat{A} \rangle = \langle\psi|\hat{A}|\psi\rangle . \tag{2.23}$$

For a system at temperature T, we find from Eqs. (2.20) and (2.21) the thermal expectation value of an observable A

$$\langle \hat{A} \rangle_\beta = \mathrm{Tr}\Big(\hat{A}\rho_\beta\Big) = \frac{\mathrm{Tr}\Big(\hat{A}e^{-\beta\hat{H}}\Big)}{\mathrm{Tr}\Big(e^{-\beta\hat{H}}\Big)}. \tag{2.24}$$

2.1.7 Simultaneous measurement of non-commuting operators

We have seen that a measurement projects a state onto an eigenvector of the operator $\hat{A}$. This projection renders commuting operators, $[\hat{A}, \hat{B}] = 0$, special, as they have the same eigenspaces and thus, can be measured successively without a further collapse of the wave function.

If, on the other hand, the operators don't commute, it is not possible to measure both observables exactly. In particular, if

$$[\hat{A}, \hat{B}] = i\hbar, \tag{2.25}$$

then the product of the root-mean-square deviations ΔA and ΔB of observables A and B fulfill

$$\Delta A \cdot \Delta B \geq \frac{\hbar}{2}. \tag{2.26}$$

The relation (2.26) is called the Heisenberg uncertainty relation. Operators that obey Eq. (2.25) are called canonically conjugate. For general operators, the right-hand side of Eq. (2.25) is still an operator, not a complex number, see for example Eqs. (2.7).

2.2 Examples

2.2.1 Single quantum particle in an external potential

The Hilbert space of wave functions in n spatial dimensions is $L_2(\mathbb{R}^n)$, the space of all twice differentiable, square-integrable, complex functions over $\mathbb{R}^n$, and is thus

infinite dimensional. Working in the coordinate representation, the position operator is given by

$$\hat{\vec{r}} = \vec{r}, \tag{2.27}$$

the scalar product is given by

$$\langle f|g\rangle = \int \mathrm{d}^n r \, f^*(\vec{r})\, g(\vec{r}), \tag{2.28}$$

and

$$\langle f|\hat{\vec{r}}|g\rangle = \int \mathrm{d}^n r \, f^*(\vec{r})\, \vec{r} g(\vec{r}). \tag{2.29}$$

The momentum operator in the real-space representation becomes

$$\hat{\vec{p}} = -i\hbar\boldsymbol{\nabla}. \tag{2.30}$$

Notice that

$$[\hat{r}_i, \hat{p}_i] = i\hbar \neq 0. \tag{2.31}$$

The Hamiltonian of the system is

$$H\left(\hat{\vec{r}}, \hat{\vec{p}}\right) = \frac{(\hat{\vec{p}})^2}{2m} + V(\hat{\vec{r}}) = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\vec{r}), \tag{2.32}$$

where the first and the second terms are the kinetic and potential energy, respectively. We then find the Schrödinger equation

$$i\hbar\frac{\partial\psi(\vec{r})}{\partial t} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\vec{r}) + V(\vec{r})\,\psi(\vec{r}). \tag{2.33}$$

2.2.2 Harmonic oscillator

A second canonical example is the (one-dimensional) harmonic oscillator with a potential $V(\hat{q}) = \frac{k}{2}\hat{q}^2$, where, as is conventional, we use the real-space coordinate q. Using units with $m = \hbar = k = 1$, the time-independent Schrödinger equation reads

$$H|n\rangle = \frac{1}{2}\left(\hat{p}^2 + \hat{q}^2\right)|n\rangle = E_n|n\rangle. \tag{2.34}$$

Inserting the definition of $\hat{p}$, we obtain an eigenvalue problem of an ordinary differential equation

$$-\frac{1}{2}\phi_n''(q) + \frac{q^2}{2}\phi_n(q) = E_n\phi_n(q) \tag{2.35}$$

with eigenfunctions

$$\phi_n(q) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}} e^{-q^2/2} H_n(q), \tag{2.36}$$

where $H_n(q)$ are the Hermite polynomials, and $n \in \mathbb{N}_0$. Finally, the eigenvalues are

$$E_n = n + 1/2. \tag{2.37}$$

There is a more elegant approach of solving this problem, motivated by the observation that $\langle m|\hat{q}|n\rangle$ and $\langle m|\hat{p}|n\rangle$ only have non-zero values for $m = n \pm 1$. In particular, we can introduce the so-called ladder operators

$$\begin{aligned} \hat{a} &= \frac{1}{\sqrt{2}}\left(\hat{q} + i\hat{p}\right), \\ \hat{a}^\dagger &= \frac{1}{\sqrt{2}}\left(\hat{q} - i\hat{p}\right) \end{aligned} \tag{2.38}$$

with commutation relations

$$\begin{aligned} [\hat{a}, \hat{a}] &= [\hat{a}^\dagger, \hat{a}^\dagger] = 0, \\ [\hat{a}, \hat{a}^\dagger] &= 1. \end{aligned} \tag{2.39}$$

The raising operator $\hat{a}^\dagger$ and the lowering operator $\hat{a}$ act as

$$\begin{aligned} \hat{a}^\dagger |n\rangle &= \sqrt{n+1}\,|n+1\rangle, \\ \hat{a}\,|n\rangle &= \sqrt{n}\,|n-1\rangle. \end{aligned} \tag{2.40}$$

Rewriting the momentum and position operators in terms of the ladder operators,

$$\begin{aligned} \hat{q} &= \frac{1}{\sqrt{2}}\left(\hat{a} + \hat{a}^\dagger\right), \\ \hat{p} &= \frac{1}{i\sqrt{2}}\left(\hat{a} - \hat{a}^\dagger\right), \end{aligned} \tag{2.41}$$

we arrive at the Hamiltonian

$$\hat{H} = \hat{a}^\dagger\hat{a} + 1/2 \tag{2.42}$$

with spectrum

$$E_n = n + 1/2, \tag{2.43}$$

as we already obtained above.

2.2.3 Spin-S problem

In section 2.1.1, we have already encountered the Hilbert space and spin operators for the most common case of a spin 1/2. The algebra of the spin operators, given by the commutation relations (2.7), allows not only for a two-dimensional representation, but for a series of $(2S+1)$-dimensional representations in a Hilbert space $\mathbb{C}^{2S+1}$ for all integer and half-integer values $S = 0, 1/2, 1, 3/2, 2, \ldots$. The basis states $\{|s\rangle\}$ are usually defined with respect to the $\hat{S}^z$ operator with the quantum number s taking values in the range $-S, -S+1, \ldots S-1, S$. These basis states are connected through

$$\begin{aligned} \hat{S}^+ |s\rangle &= \sqrt{S(S+1) - s(s+1)}\,|s+1\rangle, \\ \hat{S}^- |s\rangle &= \sqrt{S(S+1) - s(s-1)}\,|s-1\rangle, \end{aligned} \tag{2.44}$$

and

$$\begin{aligned} \hat{S}^x &= \frac{1}{2}\left(\hat{S}^+ + \hat{S}^-\right), \\ \hat{S}^y &= \frac{1}{2i}\left(\hat{S}^+ - \hat{S}^-\right). \end{aligned} \tag{2.45}$$

Finally, the dynamics of a spin coupled to a magnetic field $\vec{h}$ is given through the Hamiltonian

$$\hat{H} = -g\mu_B \vec{h} \cdot \hat{\vec{S}}. \tag{2.46}$$

3 Quantum one-body problem

3.1 Time-independent 1D Schrödinger equation

We start the numerical solution of quantum problems with the time-independent one-dimensional Schrödinger equation for a particle with mass m in a potential $V(x)$. In one dimension, the Schrödinger equation is just an ordinary differential equation

$$-\frac{\hbar^2}{2m}\partial_x^2\psi(x)+V(x)\psi(x)=E\psi(x). \tag{3.1}$$

As we already mentioned in the previous chapter, $\psi(x)$ should be twice differentiable and square-integrable, such that the wave function is normalizable,

$$\int \mathrm{d}x\,|\psi(x)|^2=1. \tag{3.2}$$

To approach this problem, we start with a simple finite-difference scheme and discretize space into intervals of length Δx, denoting the space points by

$$x_n=n\Delta x,\qquad n\in\mathbb{Z}, \tag{3.3}$$

and the wave function at these points by

$$\psi_n=\psi(x_n). \tag{3.4}$$

3.1.1 Numerov algorithm

Efficient algorithms exist for the solution of first-order ordinary differential equations, or coupled sets thereof, such as the Runge-Kutta method. One strategy to solve the second-order Schrödinger equation could thus be to rewrite it as a coupled system of two first order differential equations, and then apply such a solver. However, there exist better methods, one of which we discuss here. For the special form

$$\psi''(x)+k(x)\psi(x)=0 \tag{3.5}$$

of the Schrödinger equation, with $k(x)=2m\left(E-V(x)\right)/\hbar^2$ [and $k_n=k(x_n)$], we can derive the so-called Numerov algorithm. It starts from the Taylor expansion of ψ_n,

$$\begin{aligned}\psi_{n\pm1}=\psi_n\pm\Delta x\,\psi_n'+\frac{(\Delta x)^2}{2}\psi_n''\pm\frac{(\Delta x)^3}{6}\psi_n^{(3)}+\frac{(\Delta x)^4}{24}\psi_n^{(4)}\\ \pm\frac{(\Delta x)^5}{120}\psi_n^{(5)}+O[(\Delta x)^6],\end{aligned} \tag{3.6}$$

where $\psi_n^{(m)}$ is the m-th derivative of $\psi(x)$ evaluated at x_n. Adding ψ_{n-1} and ψ_{n+1} we obtain

$$\psi_{n-1}+\psi_{n+1}=2\psi_n+(\Delta x)^2\psi_n''+\frac{(\Delta x)^4}{12}\psi_n^{(4)}. \tag{3.7}$$

Replacing the fourth derivative by a finite-difference 'second derivative' of the second derivative

$$\psi_n^{(4)}=\frac{\psi_{n+1}''+\psi_{n-1}''-2\psi_n''}{(\Delta x)^2} \tag{3.8}$$

and substituting $-k_n\psi_n = \psi_n''$, we obtain the Numerov algorithm:

$$\left(1+\frac{(\Delta x)^2}{12}k_{n+1}\right)\psi_{n+1} = 2\left(1-\frac{5(\Delta x)^2}{12}k_n\right)\psi_n - \left(1+\frac{(\Delta x)^2}{12}k_{n-1}\right)\psi_{n-1} + O[(\Delta x)^6], \tag{3.9}$$

which is locally of sixth order in Δx.

To run the Numerov algorithm, we need the wave function not just at one point as would be the case for a first-order differential equation, but at *two* initial values. We will now present several ways to obtain these.

For potentials $V(x)$ with reflection symmetry $V(x) = V(-x)$ the wave functions need to be either even $\psi(x) = \psi(-x)$ or odd $\psi(x) = -\psi(-x)$ under reflection, which can be used to find initial values:

- For the even solution we use a mesh with half-integer mesh points $x_{n+1/2} = (n+1/2)\Delta x$ and pick initial values $\psi\left(x_{-1/2}\right) = \psi\left(x_{1/2}\right) = 1$.
- For the odd solution we know that $\psi(0) = -\psi(0)$, and hence $\psi(0) = 0$, specifying the first starting value. Using a mesh with integer mesh points $x_n = n\Delta x$ we pick $\psi(x_1) = 1$ as the second starting value.

For general potentials, we need to use other approaches. If the potential vanishes identically for large distances, i.e., $V(x) = 0$ for $|x| \geq a$, we can use the exact solution of the Schrödinger equation at large distances to define starting points, e.g.,

$$\begin{aligned}\psi(-a) &= 1,\\ \psi(-a-\Delta x) &= \exp\left(-\Delta x\sqrt{2mE}/\hbar\right).\end{aligned} \tag{3.10}$$

In the case where the potential never vanishes, we need to begin with a single starting value $\psi(x_0)$ and obtain the second starting value $\psi(x_1)$ by performing an integration over the first space step Δx with an Euler or Runge-Kutta algorithm.

Finally, at the end of the calculation, the wave function needs to be normalized.

3.1.2 1D scattering problem

The scattering problem is characterized by a potential that vanishes at large distances, $V(x) \to 0$ for $|x| \to \infty$. Its most appealing property is that solutions are guaranteed to exist for all energies $E > 0$. The solution becomes particularly simple if the potential is nonzero only on a finite interval $x \in [0, a]$, since the asymptotic solution outside of this region is a plane wave. Specifically, for a particle approaching the potential barrier from the left we can make the following ansatz for the free propagation when $x < 0$:

$$\psi_{\mathrm{L}}(x) = Ae^{iqx} + Be^{-iqx}, \tag{3.11}$$

where A is the amplitude of the incoming wave and B is the amplitude of the reflected wave. On the right hand side, once the particle has left the region of finite potential ($x > a$), we can again make a free propagation ansatz:

$$\psi_{\mathrm{R}}(x) = Ce^{iqx}. \tag{3.12}$$

The coefficients A, B and C have to be determined self-consistently by matching to a numerical solution of the Schrödinger equation in the interval $x \in [0, a]$. This is best done in the following way:

- Set $C = 1$ and use the two points a and $a+\Delta x$ as starting points for a Numerov integration.
- Numerically integrate the Schrödinger equation backwards in space, from a to 0 using the Numerov algorithm.
- Match the numerical solution of the Schrödinger equation for $x < 0$ to the free propagation ansatz (3.11) to determine A and B.

Once A and B have been determined, the reflection and transmission probabilities R and T are given by

$$R = \frac{|B|^2}{|A|^2}, \tag{3.13}$$

$$T = \frac{|C|^2}{|A|^2} = \frac{1}{|A|^2}. \tag{3.14}$$

3.1.3 Bound states and solution of the eigenvalue problem

While there exist scattering states for all energies $E > 0$, bound states solutions of the Schrödinger equation with $E < 0$ exist only for discrete energy eigenvalues (if at all). Integrating the Schrödinger equation from $-\infty$ to $+\infty$ for a negative E, we will obtain a formal solution which diverges to $\pm\infty$ as $x \to \infty$ for almost all values. These functions cannot be normalized and thus do not constitute a physical bound state solution to the Schrödinger equation. Only for discrete eigenvalues E will the solution go to zero as $x \to \pm\infty$.

A simple eigensolver can be implemented using the following shooting method, where we again will assume that the potential is zero outside an interval $[0, a]$:

- Start with an initial guess E.
- Integrate the Schrödinger equation for $\psi_E(x)$ from $x = 0$ to $x_\mathrm{f} \gg a$ and determine the value $\psi_E(x_\mathrm{f})$
- Use a root solver, such as a bisection method, to look for an energy E with $\psi_E(x_\mathrm{f}) \approx 0$.

This algorithm is not ideal since the divergence of the wave function for $x \to \pm\infty$ will cause a roundoff error that proliferates.

A better solution is to integrate the Schrödinger equation from both sides towards the center:

- Pick a starting point b and choose as energy $E = V(b)$. Note that then $\psi''_E(b) = 0$.
- Integrate both from a to b and from 0 to b. Obtain $\psi_\mathrm{L}(b)$ and $\psi_\mathrm{R}(b)$. Obtain numerical estimations for the first derivatives: $\psi'_\mathrm{L}(b) = (\psi_\mathrm{L}(b) - \psi_\mathrm{L}(b - \Delta x))/\Delta x$, $\psi'_\mathrm{R}(b) = (\psi_\mathrm{R}(b + \Delta x) - \psi_\mathrm{R}(b))/\Delta x$.

- Match the two solutions and their first derivatives at point b (matching of the second derivative we get for free, since it is zero). Keeping in mind that we can multiply non-normalized wave functions by an arbitrary factor, we obtain the conditions

$$\begin{aligned} \psi_{\mathrm{L}}(b) &= \alpha \psi_{\mathrm{R}}(b), \\ \psi'_{\mathrm{L}}(b) &= \alpha \psi'_{\mathrm{R}}(b), \end{aligned} \tag{3.15}$$

  which reduces to

$$\frac{\psi'_{\mathrm{L}}(b)}{\psi_{\mathrm{L}}(b)} = \frac{\psi'_{\mathrm{R}}(b)}{\psi_{\mathrm{R}}(b)}. \tag{3.16}$$

- Solve the last equation using any root-solving method, e.g. a bisection algorithm, to find b for which $E = V(b)$ is indeed an eigenvalue.

3.2 Time-independent Schrödinger equation in higher dimensions

The time independent Schrödinger equation in more than one dimension is a partial differential equation and cannot, in general, be solved by a simple ordinary differential equation solver such as the Numerov algorithm. Before employing a partial differential equation solver, which is substantially more difficult to handle, we should, however, first try to use symmetries to reduce the problem to decoupled one-dimensional problems. This can be done if the equation factorizes.

3.2.1 Factorization along coordinate axes

A first example is a three-dimensional Schrödinger equation in a cubic box with potential $V(\vec{r}) = V(x)\,V(y)\,V(z)$ with $\vec{r} = (x, y, z)$. Using the product ansatz

$$\psi(\vec{r}) = \psi_x(x)\,\psi_y(y)\,\psi_z(z), \tag{3.17}$$

we can factorize the partial differential equation into three independent ordinary differential equations, which can be solved as above.

3.2.2 Potential with spherical symmetry

Another factorization trick applies to spherically symmetric potentials with $V(\vec{r}) = V(|\vec{r}|)$, where an ansatz using spherical harmonics

$$\psi_{l,m}(\vec{r}) = \psi_{l,m}(r, \theta, \phi) = \frac{u(r)}{r} Y_{lm}(\theta, \phi), \quad l \in \mathbb{N}_0, \quad m \in \mathbb{Z}, \quad |m| \leq l, \tag{3.18}$$

can be used to reduce the three-dimensional Schrödinger equation to a one-dimensional one for the radial wave function $u(r)$,

$$\left(-\frac{\hbar^2}{2\mu} \frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r) \right) u(r) = E u(r), \tag{3.19}$$

where we have called the particle mass μ (to avoid confusion with magnetic quantum number m in the spherical harmonics) and $r = |\vec{r}|$. This is again a one-dimensional Schrödinger equation with a modified effective potential

$$V_l(r) = V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2} \tag{3.20}$$

and with the radial wave-function defined in the interval $r \in [0, \infty)$. Given the singular character of the potential for $r \to 0$, a numerical integration should start at large distances r and integrate towards $r = 0$, so that the largest errors are accumulated only at the last steps of the integration.

3.2.3 Finite difference methods

If we cannot use any symmetries or factorizations, we can still employ solvers for partial differential equations. One approach is to discretize the Schrödinger equation on a spatial mesh using a finite difference approximation. Replacing differentials by differences, we convert the Schrödinger equation into a system of coupled linear equations. Starting from the three-dimensional Schrödinger equation (we set $\hbar = 1$ from now on)

$$\boldsymbol{\nabla}^2 \psi(\vec{r}) + 2m\left[E - V(\vec{r})\right]\psi(\vec{r}) = 0, \tag{3.21}$$

we discretize space and obtain the system of linear equations

$$\begin{aligned} 0 = \frac{1}{(\Delta x)^2}\big[&\psi(x_{n+1}, y_n, z_n) + \psi(x_{n-1}, y_n, z_n) \\ &+\psi(x_n, y_{n+1}, z_n) + \psi(x_n, y_{n-1}, z_n) \\ &+\psi(x_n, y_n, z_{n+1}) + \psi(x_n, y_n, z_{n-1})\big] \\ &+\left\{2m\left[E - V(\vec{r})\right] - \frac{6}{(\Delta x)^2}\right\}\psi(x_n, y_n, z_n). \end{aligned} \tag{3.22}$$

Both the scattering problem and the calculation of bound states essentially reduce to eigenvalue problems. For small problems, Wolfram Mathematica or the `dsysv` function of the LAPACK library can be used. For larger problems, it is essential to realize that the matrices produced by the discretization of the Schrödinger equation are usually very sparse, meaning that only $O(N)$ of the N^2 matrix elements are nonzero. For these sparse systems of equations, optimized iterative numerical algorithms exist and are implemented in numerical libraries such as in the EIGEN library (C++) or in the SciPy module (Python). For big systems, sparse solvers such as the Lanczos algorithm (which will be discussed in detail in the following lectures) are the best and, again, there exist many efficient implementations of iterative algorithms for sparse matrices.

3.2.4 Variational approaches

There is a solution to the problem in the case of general potentials (or for more than two particles), if we are interested in the ground state and it is not possible to reduce the Schrödinger equation to a one-dimensional problem. It is based on expanding a variational wave functions in terms of a finite set of basis functions

$$|\phi\rangle = \sum_{i=1}^{N} a_i |u_i\rangle. \tag{3.23}$$

In order to estimate the ground-state energy, we want to minimize the energy E^* of the variational wave function

$$E^* = \frac{\langle\phi|\hat{H}|\phi\rangle}{\langle\phi|\phi\rangle}. \tag{3.24}$$

Since we only chose a finite basis set $\{|u_i\rangle\}$, the variational estimate E^* will always be larger than the true ground state energy E_0, but will converge towards E_0 as the size of the basis set is increased, e.g., by reducing the mesh size in a finite element basis.

To perform the minimization, we denote by

$$H_{ij} = \langle u_i|\hat{H}|u_j\rangle = \int \mathrm{d}\vec{r}\, u_i^*(\vec{r}) \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V\right) u_j(\vec{r}) \tag{3.25}$$

the matrix elements of the Hamiltonian H and by

$$S_{ij} = \langle u_i|u_j\rangle = \int \mathrm{d}\vec{r}\, u_i^*(\vec{r})\, u_j(\vec{r}) \tag{3.26}$$

the overlap matrix. Note that for an orthogonal basis set, S_{ij} is the identity matrix δ_{ij}. Minimizing Eq. (3.24) with respect to a_i^*, we obtain a generalized eigenvalue problem

$$\sum_j H_{ij}a_j = E^* \sum_k S_{ik}a_k, \tag{3.27}$$

or in a compact notation with $\vec{a} = (a_1, ..., a_N)$

$$H\vec{a} = E^* S\vec{a}, \tag{3.28}$$

where H and S are matrices consisting of H_{ij} and S_{ij} respectively. If the basis set is orthogonal, this reduces to an ordinary eigenvalue problem.

In the general case, we have to find orthogonal matrices U such that $U^{\mathrm{T}}SU$ is the identity matrix. Introducing a new vector $\vec{b} = U^{-1}\vec{a}$, we can then rearrange the problem into

$$\begin{aligned} H\vec{a} &= E^* S\vec{a}, \\ HU\vec{b} &= E^* SU\vec{b}, \\ U^T HU\vec{b} &= E^* U^T SU\vec{b} = E^*\vec{b}, \end{aligned} \tag{3.29}$$

and we end up with a standard eigenvalue problem for $U^T HU$.

Example: the anharmonic oscillator

The remaining issue is the choice of basis functions. It is advantageous to make use of known solutions to a similar problem as we will illustrate in the case of an anharmonic oscillator with the Hamiltonian

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \lambda\hat{q}^4, \\ \hat{H}_0 &= \frac{1}{2}\left(\hat{p}^2 + \hat{q}^2\right), \end{aligned} \tag{3.30}$$

where the harmonic oscillator H_0 was already discussed in Sec. 2.2.2. It makes sense to use the N lowest harmonic oscillator eigenvectors $|n\rangle$ as basis states of a finite basis and write the Hamiltonian as

$$\hat{H} = \frac{1}{2} + \hat{a}^\dagger \hat{a} + \lambda \hat{q}^4 = \frac{1}{2} + \hat{a}^\dagger \hat{a} + \frac{\lambda}{4} \left(\hat{a}^\dagger + \hat{a}\right)^4 . \tag{3.31}$$

Since the operators a and $a^\dagger$ are nonzero only in the first sub- or superdiagonal, the resulting matrix is a banded matrix with 9 nonzero bands. A sparse eigensolver, such as the Lanczos algorithm can be used to calculate the spectrum. Note that since we use the orthonormal eigenstates of H_0 as basis elements, the overlap matrix S is the identity matrix in the case at hand, reducing it to a standard eigenvalue problem.

3.2.5 Finite element method

In cases, where we have irregular geometries, want higher precision than the lowest order finite difference method, or do not know a suitable set of basis functions, the finite element method (FEM) should be chosen over the finite difference method. Explaining the FEM is a comprehensive topic in itself and we refer interested students to classes on solving partial differential equations.

3.3 Time-dependent Schrödinger equation

We are now switching to problems where we want to follow the time evolution of a given state $|\psi_0\rangle = |\psi(t_0)\rangle$, and thus study non-stationary quantum systems.

3.3.1 Spectral methods

By introducing a basis and obtaining the complete spectrum of energy eigenstates, we can directly solve the time-dependent problem in the case of a stationary (time-independent) Hamiltonian. This is a consequence of the linearity of the Schrödinger equation.

To calculate the time evolution of $|\psi_0\rangle$ from time t_0 to t, we first solve the stationary eigenvalue problem $\hat{H}|\phi\rangle = E|\phi\rangle$ and calculate the eigenvectors $|\phi_n\rangle$ with eigenvalues ε_n. Next, we represent the initial wave function $|\psi_0\rangle$ as a spectral decomposition

$$|\psi_0\rangle = \sum_n c_n |\phi_n\rangle . \tag{3.32}$$

Since each of the $|\phi_n\rangle$ is an eigenvector of $\hat{H}$, the time evolution $e^{-i\hat{H}(t-t_0)/\hbar}$ is trivial and we obtain at time t

$$|\psi(t)\rangle = \sum_n c_n e^{-i\varepsilon_n (t-t_0)/\hbar} |\phi_n\rangle . \tag{3.33}$$

This approach is, however, only useful for very small problems due to the effort of diagonalizing the Hamiltonian. A more broadly applicable method is direct numerical integration, discussed in the next two subsections.

3.3.2 Direct numerical integration

If the number of basis states is too large to perform a complete diagonalization of the Hamiltonian, or if the Hamiltonian changes over time, we need to perform a direct integration of the Schrödinger equation. Like other initial value problems of partial differential equations, the Schrödinger equation can be solved by the *method of lines*. After choosing a set of basis functions or discretizing the spatial derivatives, we obtain a set of coupled ordinary differential equations which can be evolved for each point along the time line by standard solvers for ordinary differential equations (hence the name).

A forward Euler scheme

$$|\psi(t_{n+1})\rangle = |\psi(t_n)\rangle - \frac{i\Delta t}{\hbar}\hat{H}\,|\psi(t_n)\rangle \tag{3.34}$$

is not only numerically unstable. It also violates the conservation of the norm of the wave function $\langle\psi|\psi\rangle$. Since the exact quantum evolution

$$\psi(\vec{r}, t+\Delta t) = e^{-iH\Delta t/\hbar}\psi(\vec{r}, t) \tag{3.35}$$

is unitary and thus conserves the norm, we want to look for a unitary approximant as integrator. (Here and in the remainder of this chapter we use the symbol H to denote the representation of the Hamiltonian in the chosen finite basis set.) Instead of using the forward Euler method (3.34), which is a first order Taylor expansion of the exact time evolution

$$e^{-iH\Delta t/\hbar} = \mathbb{1} - \frac{i\Delta t}{\hbar}H + O[(\Delta t)^2], \tag{3.36}$$

we reformulate the time evolution operator as

$$e^{-iH\Delta t/\hbar} = \left(e^{iH\Delta t/2\hbar}\right)^{-1} e^{-iH\Delta t/2\hbar} = \left(\mathbb{1} + \frac{i\Delta t}{2\hbar}H\right)^{-1}\left(\mathbb{1} - \frac{i\Delta t}{2\hbar}H\right) + O[(\Delta t)^3], \tag{3.37}$$

which is unitary. This gives the simplest stable and unitary integrator algorithm

$$\psi(\vec{r}, t+\Delta t) = \left(\mathbb{1} + \frac{i\Delta t}{2\hbar}H\right)^{-1}\left(\mathbb{1} - \frac{i\Delta t}{2\hbar}H\right)\psi(\vec{r}, t)\,, \tag{3.38}$$

or equivalently

$$\left(\mathbb{1} + \frac{i\Delta t}{2\hbar}H\right)\psi(\vec{r}, t+\Delta t) = \left(\mathbb{1} - \frac{i\Delta t}{2\hbar}H\right)\psi(\vec{r}, t)\,. \tag{3.39}$$

Unfortunately this is an implicit integrator: At each time step, after evaluating the right hand side a linear system of equations needs to be solved to obtain the wavefunction at the next time step. For one-dimensional problems the matrix representation of $\hat{H}$ is often tridiagonal and a tridiagonal solver can be used. In higher dimensions, the matrix H will no longer be simply tridiagonal but still very sparse and we can use iterative algorithms, similar to the Lanczos algorithm for the eigenvalue problem. For details about these algorithms (such as the biconjugate gradient (BiCG) algorithm) we refer to the summary at http://mathworld.wolfram.com/topics/Templates.html and the book "Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods" by R. Barett et al (SIAM, Philadelphia, 1994). Implementations of these algorithms are available, e.g., in the EIGEN Library for C++, or in SciPy module for Python.

3.3.3 Split operator method

A simpler and explicit method is possible for a quantum particle in the real space picture with the Schrödinger equation in continuous space. Writing the Hamiltonian as

$$\hat{H} = \hat{T} + \hat{V} \tag{3.40}$$

with

$$\hat{T} = \frac{(\hat{\vec{p}})^2}{2m}, \qquad \hat{V} = V\left(\hat{\vec{r}}\right), \tag{3.41}$$

it is easy to see that $\hat{V}$ is diagonal in position space while $\hat{T}$ is diagonal in momentum space.

Indeed, if we consider a particle in d-dimensional space, its wave function in momentum space is obtained through the Fourier transform

$$\tilde{\psi}(\vec{k}) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int_{-\infty}^{+\infty} \psi\left(\vec{r}\right) e^{-i\vec{k}\cdot\vec{r}}\, \mathrm{d}\vec{r}, \tag{3.42}$$

and the inverse Fourier transform yields

$$\psi\left(\vec{r}\right) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int_{-\infty}^{+\infty} \tilde{\psi}(\vec{k}) e^{i\vec{k}\cdot\vec{r}}\, \mathrm{d}\vec{k}\,. \tag{3.43}$$

It is then easy to check that $\tilde{\psi}(\vec{k})$ is an eigenstate of the kinetic operator $\hat{T}$, and that $\hat{T}\tilde{\psi}(\vec{k}) = \frac{\hbar^2|\vec{k}|^2}{2m}\tilde{\psi}(\vec{k})$.

If we split the time evolution as

$$e^{-i\Delta t\hat{H}/\hbar} = e^{-i\Delta t\hat{V}/2\hbar} e^{-i\Delta t\hat{T}/\hbar} e^{-i\Delta t\hat{V}/2\hbar} + O[(\Delta t)^3], \tag{3.44}$$

we can perform the individual time evolutions $e^{-i\Delta t\hat{V}/2\hbar}$ and $e^{-i\Delta t\hat{T}/\hbar}$ exactly:

$$\left\langle \vec{r}\right| e^{-i\Delta t\hat{V}/2\hbar} \left|\psi\right\rangle = e^{-i\Delta t V(\vec{r})/2\hbar} \psi\left(\vec{r}\right), \tag{3.45}$$

$$\left\langle \vec{k}\right| e^{-i\Delta t\hat{T}/\hbar} \left|\psi\right\rangle = e^{-i\Delta t\hbar\left|\vec{k}\right|^2/2m} \tilde{\psi}(\vec{k}) \tag{3.46}$$

in real space for the first term and momentum space for the second term.

Propagating for a time $t = N\Delta t$, two consecutive applications of $e^{-i\Delta t\hat{V}/2\hbar}$ can easily be combined into a propagation by a full time step $e^{-i\Delta t\hat{V}/\hbar}$, resulting in the propagation

$$\begin{aligned} e^{-it\hat{H}/\hbar} &= \left(e^{-i\Delta t\hat{V}/2\hbar} e^{-i\Delta t\hat{T}/\hbar} e^{-i\Delta t\hat{V}/2\hbar}\right)^N \\ &= e^{-i\Delta t\hat{V}/2\hbar} \left[e^{-i\Delta t\hat{T}/\hbar} e^{-i\Delta t\hat{V}/\hbar}\right]^{N-1} e^{-i\Delta t\hat{T}/\hbar} e^{-i\Delta t\hat{V}/2\hbar}. \end{aligned} \tag{3.47}$$

In practice, in order to obtain efficient representations of the wave functions both in real and momentum space, we still need to discretize real space with a suitable mesh of size Δx, for a total of P points per spatial direction. As a consequence of this discretization, the continuous Fourier transform becomes a discrete Fourier transform defined on the discrete set of wave-vectors $k_n = \frac{2\pi}{P}n$ for each spatial direction, with $n = 0, 1, ..., P-1$. Changing from real space to momentum space

then requires the application of the discrete Fourier transform and of its inverse when going back from momentum space to real space. This can be efficiently accomplished numerically thanks to the Fast Fourier Transform (FFT) algorithm, which performs the discrete Fourier transform in only $O\left(P\log\left(P\right)\right)$ operations.

The discretized algorithm then starts as

$$\begin{aligned}\psi_1\left(\vec{r}\right) &= e^{-i\Delta tV(\vec{r})/2\hbar}\psi_0\left(\vec{r}\right),\\ \tilde{\psi}_1(\vec{k}) &= \mathcal{F}\psi_1\left(\vec{r}\right),\end{aligned} \tag{3.48}$$

where $\mathcal{F}$ denotes the Fourier transform and $\mathcal{F}^{-1}$ will denote the inverse Fourier transform. Next we propagate in time using full time steps

$$\begin{aligned}\tilde{\psi}_{2n}(\vec{k}) &= e^{-i\Delta t\hbar\left|\vec{k}\right|^2/2m}\tilde{\psi}_{2n-1}(\vec{k}),\\ \psi_{2n}\left(\vec{r}\right) &= \mathcal{F}^{-1}\tilde{\psi}_{2n}(\vec{k}),\end{aligned} \tag{3.49}$$

$$\begin{aligned}\psi_{2n+1}\left(\vec{r}\right) &= e^{-i\Delta tV(\vec{r})/\hbar}\psi_{2n}\left(\vec{r}\right),\\ \tilde{\psi}_{2n+1}(\vec{k}) &= \mathcal{F}\psi_{2n+1}\left(\vec{r}\right).\end{aligned} \tag{3.50}$$

Only in the last step, we finish with another half time step in real space,

$$\psi_{2N+1}\left(\vec{r}\right) = e^{-i\Delta tV(\vec{r})/2\hbar}\psi_{2N}\left(\vec{r}\right). \tag{3.51}$$

This is a fast and unitary integrator for the Schrödinger equation in real space. It could be improved by replacing the locally third order splitting (3.44) by a fifth-order version involving five instead of three terms.

4 Introduction to the quantum many-body problem

After learning how to solve the one-body Schrödinger equation, let us next generalize to more particles. If a one-body quantum problem is described by a Hilbert space $\mathcal{H}$ of dimension $\dim(\mathcal{H}) = d$, then N *distinguishable* quantum particles are described by the tensor product of N Hilbert spaces,

$$\mathcal{H}^{(N)} = \mathcal{H}^{\otimes N} \equiv \underbrace{\mathcal{H} \otimes \mathcal{H} \otimes \cdots \otimes \mathcal{H}}_{\text{N times}} \equiv \bigotimes_{i=1}^{N} \mathcal{H} \tag{4.1}$$

with dimension d^N.

As a first example, a single spin-1/2 particle has a Hilbert space $\mathcal{H} = \mathbb{C}^2$ of dimension 2, but N spin-1/2 particles have a Hilbert space $\mathcal{H}^{(N)} = \mathbb{C}^{2^N}$ of dimension 2^N. Similarly, a single particle in three dimensions is described by a complex-valued wave function $\psi(\vec{r})$ of the position $\vec{r}$ of the particle, while N distinguishable particles are described by a complex-valued wave function $\psi(\vec{r}_1, \ldots, \vec{r}_N)$ of the positions $\vec{r}_1, \ldots \vec{r}_N$ of the particles. Approximating the Hilbert space $\mathcal{H}$ of the single particle by a finite basis set with d basis functions, the N-particle basis approximated by the same finite basis set for single particles requires d^N basis functions.

This exponential scaling of the Hilbert space dimension with the number of particles is a big (numerical) challenge. Even in the simplest case of a spin-1/2 particle with $d = 2$, the basis for $N = 32$ spins is already of size $d = 2^{32}$. A single complex vector requires 64GB of memory and will hardly fit into the memory of your PC. This challenge will be addressed during this course by learning about

1. Brute-force (exact) methods solving a problem in a huge Hilbert space for modest numbers of particles and effective (spin) models.
2. Quantum state compression to variational wave functions in the relevant part of the Hilbert space.
3. Quantum Monte Carlo methods for bosonic and magnetic systems.
4. Approximative methods, reducing the many-particle problem to a single-particle problem.

4.1 Indistinguishable particles

4.1.1 Bosons and fermions

In quantum mechanics, we assume that elementary particles, such as the electron or photon, are indistinguishable: there is no serial number painted on the electrons that would allow us to distinguish two of them. Hence, if we exchange two particles, the system is still the same as before. For a two-body wave function $\psi(\vec{r}_1, \vec{r}_2)$, where $\vec{r}$ is the particle's coordinate, this means that

$$\psi(\vec{r}_1, \vec{r}_2) = e^{i\phi}\psi(\vec{r}_2, \vec{r}_1). \tag{4.2}$$

Upon exchanging the two particles, the wave function needs to be identical up to a phase factor $e^{i\phi}$, so that all observables are invariant. Exchanging the arguments twice brings back the original wave function and can be thought of as an actual physical process in which one particle moves around the other. This path can always be contracted to a point in three dimensions [1] and thus

$$\psi\left(\vec{r}_1, \vec{r}_2\right) = e^{i\phi}\psi\left(\vec{r}_2, \vec{r}_1\right) = e^{2i\phi}\psi\left(\vec{r}_1, \vec{r}_2\right). \tag{4.3}$$

As a consequence, $e^{i\phi} = \pm 1$ and

$$\psi\left(\vec{r}_1, \vec{r}_2\right) = \pm\psi\left(\vec{r}_2, \vec{r}_1\right). \tag{4.4}$$

The many-body Hilbert space can be split into two orthogonal subspaces: one in which particles pick up a '$-$' sign upon exchange of any two particles and are called *fermions*, and the other where particles pick up a '$+$' sign and are called *bosons*.

Bosons

For bosons, the general many-body wave function needs to be symmetric under permutations. Instead of an arbitrary wave function $\psi\left(\vec{r}_1, \ldots \vec{r}_N\right)$ of N particles, we use the symmetrized wave function

$$\Psi^{(\mathrm{S})} = \mathcal{S}_+\psi\left(\vec{r}_1, \ldots \vec{r}_N\right) \equiv \mathcal{N}_{\mathrm{S}} \sum_p \psi\left(\vec{r}_{p(1)}, \ldots, \vec{r}_{p(N)}\right), \tag{4.5}$$

where the sum runs over all permutations p of N particles, and $\mathcal{N}_{\mathrm{S}}$ is a normalization factor.

Fermions

For fermions, the wave function has to be antisymmetric under exchange of any two fermions, and we use the antisymmetrized wave function

$$\Psi^{(\mathrm{A})} = \mathcal{S}_-\psi\left(\vec{r}_1, \ldots \vec{r}_N\right) \equiv \mathcal{N}_{\mathrm{A}} \sum_p \mathrm{sign}\left(p\right) \psi\left(\vec{r}_{p(1)}, \ldots, \vec{r}_{p(N)}\right), \tag{4.6}$$

where $\mathrm{sign}\left(p\right) = \pm 1$ is the sign of the permutation and $\mathcal{N}_{\mathrm{A}}$ again is a normalization factor.

A 'consequence' of the antisymmetrization is the *Pauli exclusion principle*, which states that no two fermions can occupy the same state $\phi(\vec{r})$,

$$\psi\left(\vec{r}_1, \vec{r}_2\right) = \phi\left(\vec{r}_1\right)\phi\left(\vec{r}_2\right), \tag{4.7}$$

since this vanishes under antisymmetrization,

$$\Psi\left(\vec{r}_1, \vec{r}_2\right) \propto \psi\left(\vec{r}_1, \vec{r}_2\right) - \psi\left(\vec{r}_2, \vec{r}_1\right) = \phi\left(\vec{r}_1\right)\phi\left(\vec{r}_2\right) - \phi\left(\vec{r}_2\right)\phi\left(\vec{r}_1\right) = 0. \tag{4.8}$$

Note that here and in the following, we have dropped the superscript A (or S), since it should always be clear what particles we are talking about.

[1] In two dimensions, it matters whether we move the particles clockwise or anticlockwise when exchanging them, and two clockwise exchanges are not necessarily an identity anymore. Then, more generally, anyonic statistics is possible.

Spinful fermions

Fermions, such as electrons, usually have a spin-1/2 degree of freedom in addition to their orbital wave function. The full wave function as a function of a generalized coordinate $r = (\vec{r}, \sigma)$ including both position $\vec{r}$ and spin σ has to be antisymmetric.

4.1.2 Fock space

The Hilbert space describing a quantum many-body system with $N = 0, 1, \ldots, \infty$ particles is called the Fock space. It is the direct sum of the appropriately symmetrized N-particle Hilbert spaces $\mathcal{H}^{\otimes N}$,

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{S}_{\pm} \mathcal{H}^{\otimes N}, \tag{4.9}$$

where $\mathcal{S}_+$ is the symmetrization operator used for bosons and $\mathcal{S}_-$ is the antisymmetrization operator used for fermions.

Occupation number basis

Given a basis $\{|\phi_1\rangle, \ldots, |\phi_N\rangle\}$ of the single-particle Hilbert space $\mathcal{H}$, a basis for the Fock space is constructed by specifying the number of particles n_i occupying the single-particle state $|\phi_i\rangle$. The wave function of the state $|n_1, \ldots, n_N\rangle$ is given by the appropriately symmetrized and normalized product of the single-particle wave functions. For example, the state $|1, 1\rangle$ corresponds to the wave function

$$\frac{1}{\sqrt{2}} \left[\phi_1(r_1)\, \phi_2(r_2) \pm \phi_1(r_2)\, \phi_2(r_1)\right], \tag{4.10}$$

where again the $+$ sign is for bosons and the $-$ sign is for fermions.

For bosons, the occupation numbers n_i can go from 0 to ∞, while for fermions they are restricted to $n_i = 0$ or 1, since no two fermions can occupy the same state.

Slater determinant

The antisymmetrized and normalized product of N single-particle wave functions ϕ_i can be written as a determinant, called the Slater determinant,

$$\Psi(r_1, \ldots, r_N) = \mathcal{S}_- \prod_{i_1}^{N} \phi_i(r_i) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(r_1) & \ldots & \phi_N(r_1) \\ \vdots & & \vdots \\ \phi_1(r_N) & \ldots & \phi_N(r_N) \end{vmatrix}. \tag{4.11}$$

Note that while the set of Slater determinants of single-particle basis functions forms a basis of the fermionic Fock space, the general fermionic many-body wave function is a linear superposition of many Slater determinants and cannot be written as a single Slater determinant. The Hartee-Fock method, discussed below, will simplify the quantum many-body problem to a one-body problem by making the approximation that the ground-state wave function can be described by a single Slater determinant.

4.1.3 Creation and annihilation operators

Since it is very cumbersome to work with appropriately symmetrized many-body wave functions, we will mainly use the formalism of second quantization and work with creation and annihilation operators.

The annihilation operator a_i associated with a basis function $|\phi_i\rangle$ is defined as the result of the inner product of a many-body wave function $|\Psi\rangle$ with this basis function $|\phi_i\rangle$. Given an N-particle wave function $|\Psi^{(N)}\rangle$, the result of applying the annihilation operator is an $(N-1)$-particle wave function $|\tilde{\Psi}^{(N-1)}\rangle = \hat{a}_i |\Psi^{(N)}\rangle$. It is given by the appropriately symmetrized inner product

$$\tilde{\Psi}(r_1, \ldots, r_{N-1}) = \mathcal{S}_{\pm} \int \mathrm{d}r_N \, \phi_i^*(r_N) \, \Psi(r_1, \ldots, r_N) \,. \tag{4.12}$$

Applied to a single-particle basis state $|\phi_j\rangle$, the result is

$$\hat{a}_i |\phi_j\rangle = \delta_{ij} |0\rangle \,, \tag{4.13}$$

where $|0\rangle$ is the "vacuum" state with no particles.

The creation operator $\hat{a}_i^\dagger$ is defined as the adjoint of the annihilation operator $\hat{a}_i$. Applying it to the vacuum "creates" a particle with the wave function

$$|\phi_i\rangle = \hat{a}_i^\dagger |0\rangle \,. \tag{4.14}$$

For the sake of simplicity and concreteness, we will in general assume that the N basis functions $|\phi_i\rangle$ of the single-particle Hilbert space factor into $N/(2S+1)$ orbital wave functions $f_i(\vec{r})$ and $2S+1$ spin wave functions $|\sigma\rangle$, where $\sigma = -S, -S+1, \ldots, S$. We will write creation and annihilation operators $\hat{a}_{i,\sigma}^\dagger$ and $\hat{a}_{i,\sigma}$, where i is the orbital index and σ is the spin index. The most common cases will be spinless bosons with $S = 0$, where the spin index can be dropped and spin-1/2 fermions, where the spin can be up $(+1/2)$ or down $(-1/2)$.

Commutation relations

The creation and annihilation operators satisfy certain canonical commutation relations, which we will discuss for an orthogonal set of basis functions.

For bosons, the commutation relations are the same as those of the ladder operators discussed for the harmonic oscillator, Eq. (2.39), namely

$$\begin{aligned} [\hat{a}_i, \hat{a}_j^\dagger] &= \hat{a}_i \hat{a}_j^\dagger - \hat{a}_j^\dagger \hat{a}_i = \delta_{ij}, \\ [\hat{a}_i, \hat{a}_j] &= [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0. \end{aligned} \tag{4.15}$$

For fermions, on the other hand, the operators anticommute,

$$\begin{aligned} \{\hat{a}_i, \hat{a}_j^\dagger\} &= \hat{a}_i \hat{a}_j^\dagger + \hat{a}_j^\dagger \hat{a}_i = \delta_{ij}, \\ \{\hat{a}_i, \hat{a}_j\} &= \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0. \end{aligned} \tag{4.16}$$

The anticommutation implies that

$$(\hat{a}_i^\dagger)^2 = \hat{a}_i^\dagger \hat{a}_i^\dagger = -\hat{a}_i^\dagger \hat{a}_i^\dagger, \tag{4.17}$$

and thus guarantees that

$$(\hat{a}_i^\dagger)^2 = 0, \tag{4.18}$$

as expected from the Pauli exclusion principle.

Fock basis in second quantization and normal ordering

The basis state $|n_1, \ldots, n_N\rangle$ in the occupation-number basis can easily be expressed in terms of creation operators

$$|n_1, \ldots, n_N\rangle = \prod_{i=1}^{N} (\hat{a}_i^\dagger)^{n_i} |0\rangle = (\hat{a}_1^\dagger)^{n_1} (\hat{a}_2^\dagger)^{n_2} \ldots (\hat{a}_N^\dagger)^{n_N} |0\rangle . \tag{4.19}$$

For bosons, the ordering of the creation operators does not matter, since the operators commute. For fermions, however, the ordering matters since the fermionic creation operators anticommute and $\hat{a}_1^\dagger \hat{a}_2^\dagger |0\rangle = -\hat{a}_2^\dagger \hat{a}_1^\dagger |0\rangle$. We therefore need to agree on a specific ordering of the creation operators to define what we mean by the state $|n_1, \ldots, n_N\rangle$. The choice of ordering does not matter but we have to stay consistent and use, e.g., the convention in Eq. (4.19).

Once the normal ordering is defined, we can derive the expressions for the matrix elements of the creation and annihilation operators in that basis. Using above normal ordering, the matrix elements are

$$\begin{aligned} \hat{a}_i |n_1, \ldots, n_i, \ldots, n_N\rangle &= \delta_{n_i,1} (-1)^{\sum_{j=1}^{i-1} n_j} |n_1, \ldots, n_i - 1, \ldots, n_N\rangle , \\ \hat{a}_i^\dagger |n_1, \ldots, n_i, \ldots, n_N\rangle &= \delta_{n_i,0} (-1)^{\sum_{j=1}^{i-1} n_j} |n_1, \ldots, n_i + 1, \ldots, n_N\rangle , \end{aligned} \tag{4.20}$$

where the minus signs stem from commuting the annihilation and creation operator to the correct position in the normal ordered product.

4.2 Quantum spin models

In the study of many-body systems, we are interested in complex phase diagrams or quantum dynamics. Of particular interest are quantum phase transitions, in other words phase transitions driven by quantum, not thermal, fluctuations. As only very few problems allow for an exact solution and the complexity of the Hilbert space severely restricts numerically tackling complicated models, we need to find model systems capturing a broad range of complex phenomena while being as simple as possible.

In (classical) statistical mechanics, the Ising model and other idealized (spin) models have allowed for insights into thermal phase transitions, their universality, and critical phenomena. In order for a model to exhibit quantum phenomena, an extensive number of operators of the model Hamiltonian must not commute with each other. Again, this can be realized in 'simple' spin models, since the spin operators defined in Sec. 2.1.2 indeed satisfy a non-trivial algebra. Quantum spin models are thus instrumental in investigating exotic quantum many-body states and quantum phase transitions. Finally, interacting fermions can in principle be mapped to spin models, though in practice, this is mainly restricted to one-dimensional systems.

4.2.1 Transverse field Ising model

The Drosophila of quantum spin models is the transverse field Ising model (TFIM), which exhibits a quantum phase transition between a spontaneously symmetry-broken and a disordered phase. It derives from the classical Ising model, a model

describing a lattice of spin-1/2 particles coupled only through their spins' z component, by adding a magnetic field in the x direction,

$$\hat{H} = -\sum_{\langle ij \rangle} J_{ij} \hat{S}_i^z \hat{S}_j^z - \sum_i \frac{h_i}{2} \hat{S}_i^x. \tag{4.21}$$

Here, the symbol $\langle ij \rangle$ denotes a sum over all nearest-neighbor bonds in the lattice (without double-counting). Note that $\langle\langle ij \rangle\rangle$ would denote next-nearest neighbors. In this model, the spin operator for the x component does not commute with the z component, rendering this model inherently quantum.

For the translationally invariant one-dimensional case, in other words $J_{ij} = J$, $h_i = h$, this model is exactly solvable and exhibits a $T = 0$ phase diagram as shown in Fig. 3.

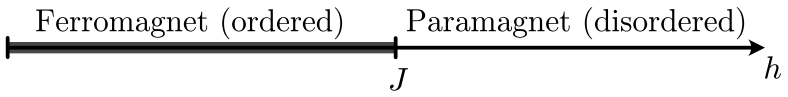


Figure 3: Zero temperature phase diagram of the Transverse field Ising model.

4.2.2 The Heisenberg model

The (quantum) Heisenberg model is the generalization of the classical Heisenberg model to non-commuting spin operators,

$$\hat{H} = \sum_{\langle ij \rangle} J_{ij} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j = \sum_{\langle ij \rangle} J_{ij} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \hat{S}_i^z \hat{S}_j^z \right). \tag{4.22}$$

We can introduce raising and lowering operators $\hat{S}^+$ and $\hat{S}^-$ as in Eq. (2.45) to find

$$\hat{H} = \sum_{\langle ij \rangle} J_{ij} \left[\frac{1}{2} \left(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+ \right) + \hat{S}_i^z \hat{S}_j^z \right]. \tag{4.23}$$

The three terms in Eq. (4.23) clearly do not change the *total* magnetization $\hat{M}^z = \sum_i \hat{S}_i^z$, in other words $\hat{M}^z$ is a symmetry of the Heisenberg Hamiltonian. Note that the first two terms can change the magnetization locally. What is more, the Heisenberg Hamiltonian possesses SU(2) symmetry, meaning it commutes with the operator $\exp\left(i\vec{\theta} \cdot \hat{\vec{M}}\right)$, where $\vec{\theta}$ is an arbitrary vector and $\hat{\vec{M}} = (\hat{M}^x, \hat{M}^y, \hat{M}^z) = \left(\sum_i \hat{S}_i^x,\ \sum_i \hat{S}_i^y,\ \sum_i \hat{S}_i^z \right)$. [2]

Using the basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ for two spins, the matrix representation of the two-site operator is

$$\begin{pmatrix} J_{ij}/4 & 0 & 0 & 0 \\ 0 & -J_{ij}/4 & J_{ij}/2 & 0 \\ 0 & J_{ij}/2 & -J_{ij}/4 & 0 \\ 0 & 0 & 0 & J_{ij}/4 \end{pmatrix}. \tag{4.24}$$

The block-diagonal form reflects the conservation of the total magnetization.

[2] This is equivalent to the Hamiltonian commuting with $\hat{M}^x, \hat{M}^y, \hat{M}^z$.

4.2.3 The XXZ model

Typically, magnetic materials do not have the full SU(2) symmetry, but possess an easy axis or an easy plane for the spins. Such preferred directions are captured by the so-called XXZ model described by the Hamiltonian

$$\hat{H} = J \sum_{\langle ij \rangle} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \Delta \hat{S}_i^z \hat{S}_j^z \right). \tag{4.25}$$

For an *anisotropy* $\Delta = 0$, we find the quantum XY model, for $\Delta = 1$ we have the Heisenberg model, while for $\Delta \to \infty$, we recover the Ising model. Note that all these models conserve the total magnetization $\hat{M}^z$.

4.2.4 Mapping of spin models to (spinless) fermions in 1D

The raising and lowering operators $\hat{S}^{\pm} = \hbar\sigma^{\pm}$ satisfy $(\sigma_i^+)^2 = 0$, in other words a spin can be flipped only once; attempting to flip it twice annihilates the state. This property resembles the Pauli principle for fermions, where acting with the same operator twice anihiliates any state. Even though there is a fundamental difference in the operators acting on different sites of a spin system and a fermionic system, namely the commutation relations of the operators, we can map the above introduced spin models to (spinless) fermions in one dimension. The mapping that achieves this and takes care of the right commutation relations is the Jordan-Wigner transformation and is given by

$$\hat{c}_i = \prod_{j<i} \left(-\sigma_j^z\right) \sigma_i^-, \tag{4.26}$$

and

$$\hat{c}_i^\dagger = \prod_{j<i} \left(-\sigma_j^z\right) \sigma_i^+. \tag{4.27}$$

One checks that the so-defined operators satisfy

$$\{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij}, \qquad \{\hat{c}_i, \hat{c}_j\} = \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0, \tag{4.28}$$

i.e., they furnish a Hilbert space of a chain with one fermionic degree of freedom per site. Notice that the fermionic operators, when written in terms of the spin operators are *non-local*. This non-locality is necessary to build in the fermionic anticommutation relations and caused by the "string" operator

$$\hat{K}_i = \prod_{j<i} \left(-\sigma_j^z\right), \tag{4.29}$$

which accounts for commuting through the operators to the position i, see also Eq. (4.20).

Using this transformation, the XXZ model becomes (up to chemical potential and constant terms)

$$\hat{H} = \frac{J}{2} \sum_{\langle ij \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + h.c. + 2\Delta \hat{n}_i \hat{n}_j \right) \tag{4.30}$$

with $\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$, which describes (spinless) fermions hopping on a chain subject to a nearest-neighbor interaction $U = J\Delta$. Note how the conserved magnetization $\hat{M}^z$ of the XXZ model is mapped to a conserved particle number $\hat{N} = \sum_i \hat{n}_i$.

Note that we are often interested in simulating fermions. In order to avoid dealing with the anticommutating operators of the fermionic model, we usually map the Hamiltonian to a spin model. For a 1D system with operators that have only local support, the resulting Hamiltonian is always also local.

5 Exact diagonalization methods

After we got acquainted with various (spin-1/2) model systems in the last chapter, we now want to calculate their properties. In this chapter, we learn about exact diagonalization methods for finding the ground state (or a few lowest states) and for the time evolution of a given initial state. For a system of size N, the Hilbert space has dimension 2^N and thus, the Hamiltonian is a matrix of dimension $2^N \times 2^N$. Therefore, only very small system sizes—usually in one dimension—can be tackled. While exact diagonalization approaches are very useful for benchmarking more elaborate methods and sometimes are even the only method available, care has to be taken when interpreting the results in terms of a thermodynamic limit.

5.1 Exact Diagonalization

The most accurate method is completely diagonalizing the Hamiltonian matrix. If we want to obtain the full spectrum, only system sizes $N \sim 20$ are reachable. If we are only interested in the ground state or a few lowest-energy states, we can use iterative solvers, in particular the Lanczos algorithm, which allow system sizes $N \sim 40$. This is usually referred to as *exact diagonalization* or ED.

5.1.1 Lanczos Algorithm

To motivate the Lanczos algorithm, we will first take a look at the power method for a matrix A. For concreteness, we will use the Hamiltonian H as the matrix. Then, we start from a random vector

$$\vec{v} = \sum_n c_n \vec{n} \tag{5.1}$$

with $H\vec{n} = \lambda_n \vec{n}$. Applying the Hamiltonian to $\vec{v}$, we find

$$H\vec{v} = \sum_n c_n \lambda_n \vec{n} \tag{5.2}$$

and repeating this process M times, we obtain vectors

$$\vec{v}_k := H^k \vec{v} = \sum_n c_n \lambda_n^k \vec{n}, \qquad k = 0, 1, 2, \ldots, M. \tag{5.3}$$

If λ_{n_0} is the largest eigenvalue (with non-zero coefficient c_{n_0}), we can rewrite

$$\vec{v}_M = c_{n_0} (\lambda_{n_0})^M \left[\vec{n_0} + \sum_{n \neq n_0} \frac{c_n}{c_{n_0}} \left(\frac{\lambda_n}{\lambda_{n_0}} \right)^M \vec{n} \right]. \tag{5.4}$$

For $M \to \infty$, this procedure, thus, converges (slowly) to the state with the largest eigenvalue. The Lanczos algorithm optimizes this crude method.

The (normalized) vectors $\vec{v}_k$ span the *Krylov* space

$$K_M = \text{span} \left\{ \frac{\vec{v}}{\|\vec{v}\|}, \frac{H\vec{v}}{\|H\vec{v}\|}, \frac{H^2\vec{v}}{\|H^2\vec{v}\|}, \ldots, \frac{H^M\vec{v}}{\|H^M\vec{v}\|} \right\}. \tag{5.5}$$

Next, we orthogonalize the basis vectors employing a *Gram-Schmidt orthogonalization*

$$\begin{aligned}
&\vec{r}_0 = \vec{v}/\|\vec{v}\|,\\
&\beta_1\vec{r}_1 = H\vec{r}_0 - \alpha_0\vec{r}_0,\\
&\beta_2\vec{r}_2 = H\vec{r}_1 - \alpha_1\vec{r}_1 - \beta_1\vec{r}_0,\\
&\dots\\
&\beta_{n+1}\vec{r}_{n+1} = H\vec{r}_n - \alpha_n\vec{r}_n - \beta_n\vec{r}_{n-1},\\
&\dots\\
&\beta_M\vec{r}_M = H\vec{r}_{M-1} - \alpha_{M-1}\vec{r}_{M-1} - \beta_{M-1}\vec{r}_{M-2},
\end{aligned} \tag{5.6}$$

where

$$\begin{aligned}
\alpha_n &= \vec{r}_n^\dagger H\vec{r}_n,\\
\beta_n &= \left|\vec{r}_n^\dagger H\vec{r}_{n-1}\right|.
\end{aligned} \tag{5.7}$$

This yields an orthonormal basis with $\vec{r}_n^\dagger\vec{r}_m = \delta_{nm}$. As the orthogonality condition does not determine the phases of the basis vectors, β_n can be chosen to be real and positive. Expressed in this basis, the Hamiltonian H is a tridiagonal matrix

$$H^{(M)} \equiv \begin{pmatrix}
\alpha_0 & \beta_1 & 0 & \dots & 0\\
\beta_1 & \alpha_1 & \ddots & \ddots & \vdots\\
0 & \ddots & \ddots & \ddots & 0\\
\vdots & \ddots & \ddots & \ddots & \beta_M\\
0 & \dots & 0 & \beta_M & \alpha_M
\end{pmatrix}. \tag{5.8}$$

The eigenvalues of $H^{(M)}$ provide a good approximation of the eigenvalues of the Hamiltonian H, with the extremal eigenvalues converging very fast, such that $M \ll 2^N$ steps are required. Note that $H^{(M)}$ is only a $(M+1)\times(M+1)$ matrix, so it is easy to diagonalize and check for convergence. Furthermore, for the construction of the Hamiltonian, we only need to store three vectors of size 2^N in memory, which makes the Lanczos algorithm very efficient when compared to dense matrix eigensolvers which requires storage of order $(2^N)^2$. Furthermore, note that we do not need the explicit form of the Hamiltonian; the Lanczos algorithm only needs a linear operator, in other words the rules for matrix multiplication with H, $H : \vec{v} \mapsto H\vec{v}$ as an input. This allows for an extremely efficient implementation of matrix-vector multiplication for spin Hamiltonians, as we will discuss below.

It is also straight forward to compute the eigenvectors of $H^{(M)}$. They are, however, given in the Lanczos basis $\{\vec{r}_n\}$. To obtain the eigenvectors in the original basis we need to perform a basis transformation. Due to memory constraints we usually do not store all the $\vec{r}_n$, but only the last three vectors. To transform the eigenvector to the original basis we have to do the Lanczos iterations a second time. Starting from the same initial vector $\vec{r}_0$ we construct the vectors $\vec{r}_n$ iteratively and perform the basis transformation as we go along.

One problem that we need to be aware of: in principle all Lanczos vectors $\vec{r}_n$ are orthogonal to each other. But round-off errors spoil this property, and "new" low-lying eigenvalues appear throughout the iteration. These are called *ghost states* and have to be removed.

Numerically stable and efficient implementations of the Lanczos algorithm can be obtained as part of open-source packages (EIGEN library for C++, scipy.linalg module for Python).

5.1.2 Spin-1/2 Hamiltonians

A straight forward implementation of a spin Hamiltonian can be achieved using direct products of spin operators. For this purpose, we add identity matrices on all sites outside the operator's support. For the example of an Ising term, we can write in matrix form

$$\hat{S}_i^z \hat{S}_{i+1}^z = \underbrace{\mathbb{1}}_{n=1} \otimes \cdots \otimes \underbrace{\mathbb{1}}_{n=i-1} \otimes \underbrace{\hat{S}^z}_{n=i} \otimes \underbrace{\hat{S}^z}_{n=i+1} \otimes \underbrace{\mathbb{1}}_{n=i+2} \cdots . \tag{5.9}$$

As noted above, for a system of length N, the total Hamiltonian matrix has $O(2^N \times 2^N)$ terms, a prohibitively large number for "large" N. The good news is that all (spin) Hamiltonians introduced in the previous section contain only $O(N^2)$ two-body terms. As a consequence, most of the matrix elements of the Hamiltonian matrix are zero. However, even the storage of a sparse matrix with $O(N^2 2^N)$ matrix elements is prohibitive for large N. Here, the Lanczos algorithm again provides a route forward: For the algorithm's application, the full matrix is never necessary, but only the action of H on a state $\vec{v}$. What we need then are (1) a representation of the basis states suited for the problem and (2) an efficient way of calculating $H\vec{v}$.

The 2^N basis states of a quantum spin-1/2 system can simply be represented as N-bit strings. To do so, we represent every basis state by a single integer between $0, \ldots, 2^N - 1$. The value of the i-th bit of the integer corresponds to the orientation of the i-th spin in that configuration: A value of 0 denotes a $\downarrow$ spin, while 1 corresponds to $\uparrow$. For $N = 3$, the basis states then are

$$\{|\{s_i\}\rangle\} = \{\underset{0=000_2}{|\downarrow\downarrow\downarrow\rangle}, \underset{1=001_2}{|\downarrow\downarrow\uparrow\rangle}, \underset{2=010_2}{|\downarrow\uparrow\downarrow\rangle}, \underset{3=011_2}{|\downarrow\uparrow\uparrow\rangle}, \underset{4=100_2}{|\uparrow\downarrow\downarrow\rangle}, \underset{5=101_2}{|\uparrow\downarrow\uparrow\rangle}, \underset{6=110_2}{|\uparrow\uparrow\downarrow\rangle}, \underset{7=111_2}{|\uparrow\uparrow\uparrow\rangle}\}. \tag{5.10}$$

Using these basis states, an efficient implementation of the Hamiltonian requires only bitwise operations. As an example, we discuss the Heisenberg model. We can implement the diagonal term $\hat{S}_i^z \hat{S}_{i+1}^z$ using an XOR between the original state s and the state with all bits shifted by one, $\tilde{s}$. In Python code this would be `s_tilde = s ^ (s>>1)`. For each aligned pair of spins, this will set a bit to 0, while for antialigned spins, this sets a bit to 1. For example, using the state $s = 3 = 011_2$, we find for $\tilde{s} = 011_2 \,\hat{}\, 001_2 = 010_2$. Now we can simply count the number of bits 0 and 1 in $\tilde{s}$ to determine the diagonal matrix value of the state s. Similarly, for the $\hat{S}_i^+ \hat{S}_{i+1}^- + \text{h.c.}$ term, we can use $\tilde{s}$ and if a bit is set at position r, then we flip the two neighboring spins by an XOR operation of s with `s_new = s ^ (3<<r)`. The Hamiltonian then has a matrix element between s and s_{new} with matrix element $J/2$.

5.1.3 Symmetries

If a Hamiltonian obeys some symmetries, such as total magnetization, particle number, or momentum, we can block diagonalize the Hamiltonian and solve within the

symmetries' eigenspaces. As an example, we discuss in the following the Transverse Field Ising Model, for which we can define a parity operation $\hat{P}$ through

$$\hat{P} = \prod_i \sigma_i^x, \tag{5.11}$$

which is a symmetry of $\hat{H}$, meaning

$$[\hat{P}, \hat{H}] = 0. \tag{5.12}$$

Furthermore, applying parity twice yields the original state,

$$\hat{P}^2 = \mathbb{1}. \tag{5.13}$$

From Eq. (5.13), it follows that the parity operator has eigenvalues $P = \pm 1$. Working in an eigenbasis $|\alpha_\pm\rangle$ of $\hat{P}$, all matrix elements between the two eigenspaces vanish, since for any two states $|+\rangle$ and $|-\rangle$,

$$\langle +|\hat{H}|-\rangle = \langle +|\hat{P}\hat{H}|-\rangle = \langle +|\hat{H}\hat{P}|-\rangle = -\langle +|\hat{H}|-\rangle = 0. \tag{5.14}$$

Implementation

To make use of a symmetry $\hat{S}$, we need to:

1. Find the eigenspaces of the symmetry operator $\hat{S}$ and an appropriate basis. For this purpose, we start from each basis state and apply $\hat{S}$ exactly M times until we find the initial state again. The set of states related by the symmetry is called an orbit. Note that for $\hat{P}$, $M = 2$. For each eigenspace of the symmetry, we construct eigenfunctions out of these orbits (if possible) and denote them by a representative and the eigenvalue. For the case of $N = 3$ and parity, for example, we find the orbits

$$\{|\uparrow\uparrow\uparrow\rangle, |\downarrow\downarrow\downarrow\rangle\}, \{|\uparrow\uparrow\downarrow\rangle, |\downarrow\downarrow\uparrow\rangle\}, \{|\uparrow\downarrow\uparrow\rangle, |\downarrow\uparrow\downarrow\rangle\}, \{|\downarrow\uparrow\uparrow\rangle, |\uparrow\downarrow\downarrow\rangle\} \tag{5.15}$$

   and we can construct eigenstates such as

$$|\downarrow\downarrow\downarrow, \pm\rangle = \frac{1}{\sqrt{2}}\big(|\downarrow\downarrow\downarrow\rangle \pm |\uparrow\uparrow\uparrow\rangle\big). \tag{5.16}$$

2. Construct the Hamiltonian in the eigenspaces. Note that if we want to only define a linear operator (instead of an explicit Hamiltonian matrix), fast look-up tables that map an index to a representative, find the representative of a given state in an orbit, and find the index of a representative are essential.

5.1.4 Symmetries example: Basis for the given magnetization sector

In the XXZ and Heisenberg model conservation of the total magnetization allows us to restrict the diagonalization to a subspace of fixed magnetization. These states have a fixed number of $N/2 + M^z$ spin-$\uparrow$ and $N/2 - M^z$ spin-$\downarrow$. These states can hence be characterized by all N-bit bit strings that have $N/2 - M^z$ bits set to 1. Our code now cannot just use the integers $0 \ldots 2^N - 1$ to enumerate the states, but we can write a small class to map an index to the bit string of a state and back.

In the code fragment below we use the following variables:

- `states_` is a vector storing the integers whose bit pattern correspond to the basis states. It can be accessed using the following functions:
  - `dimension()` returns the number of basis states.
  - `state(i)` returns the i-th basis state, where i runs from 0 to `dimension`()−1.
- `index_` is a much larger vector of size 2^N. It is used to obtain the number of a state in the basis, given the integer representation of the state. It can be accessed using the function
  - `index(s)` which returns the index i of the state in the basis, or the largest integer to denote an invalid state, if the bit pattern of the integer does not correspond to a basis state.

  Since this vector is very large, it will limit the size of systems that can be studied. To save space, the `index_` array could be omitted and the `index(s)` function implemented by a binary search on the `states_` array.

Here is the C++ code for this class:

```
class FixedMagnetizationBasis {
public:
  typedef unsigned int state_type;
  typedef unsigned int index_type;
  FixedMagnetizationBasis (int N, int Ndown);

  state_type state(index_type i) const {return states_[i];}
  index_type index(state_type s) const {return index_[s];}
  index_type dimension() const { return states_.size();}

private:
  std::vector<state_type> states_;
  std::vector<index_type> index_;
};
```

In the constructor we build the basis states. The constructor uses the `alps::popcnt` function of the ALPS library that counts the number of zeros in a binary representation of an integer.

```
  FixedMagnetizationBasis::FixedMagnetizationBasis (int N, int Ndown)
  : index_(1<<N); // 2^N entries
{
  for (state_type s=0;s<index_.size();++s)
    if(alps::popcnt(s)==Ndown) {  // correct number of down-spins
          states_.push_back(s);
          index_[s]=states_.size()-1;
    }
    else
      // invalid state
      index_[s]=std::numeric_limits<index_type>::max();
}
```

5.2 Time evolution

As for the single-particle case, we want to solve the time evolution of some initial state, governed by

$$i\hbar\partial_t |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle \tag{5.17}$$

both for constant Hamiltonians $\hat{H}(t) \equiv \hat{H}$ and for time-dependent ones.

5.2.1 Time-independent Hamiltonians

The exact solution to Eq. (5.17) can be obtained by integration, namely

$$|\psi(t + \Delta t)\rangle = e^{-i\hat{H}\Delta t/\hbar} |\psi(t)\rangle . \tag{5.18}$$

However, the exponential of the sparse matrix is dense, rendering this computationally too costly. Unfortunately, as we have seen in the case of the single-particle time evolution, simply expanding the exponential leads to non-unitary time evolution. In the case of single-particle time evolution with $\hat{H} = \hat{T} + \hat{V}$, we discussed the split-operator method, where $e^{\hat{O}}$ for some operator $\hat{O}$ can be applied exactly. Here, we go along a similar line.

Trotter-Suzuki decomposition

We split the Hamiltonian into a sum of K terms that mutually don't commute,

$$\hat{H} = \sum_{k=1}^{K} \hat{h}_k, \tag{5.19}$$

but which we know how to exponentiate explicitly. We then decompose the time-evolution operator for a small time step Δt into multiple products of the non-commuting terms in the Hamiltonian using the Baker-Campbell-Hausdorff formula. To first order, we have

$$e^{-i\hat{H}\Delta t/\hbar} = \prod_{k=1}^{K} e^{-i\hat{h}_k\Delta t/\hbar} + O\left((\Delta t)^2\right) . \tag{5.20}$$

The second-order version reads

$$e^{-i\hat{H}\Delta t/\hbar} = \hat{S}\left(\frac{\Delta t}{2}\right) + O\left((\Delta t)^3\right) , \tag{5.21}$$

where

$$\hat{S}\left(\Delta t\right) = \left(\prod_{k=1}^{K} e^{-i\hat{h}_k\Delta t/\hbar}\right)\left(\prod_{k=K}^{1} e^{-i\hat{h}_k\Delta t/\hbar}\right) . \tag{5.22}$$

For $K = 2$, this simplifies to

$$e^{-i\hat{H}\Delta t/\hbar} = e^{-i\hat{h}_1\Delta t/2\hbar} e^{-i\hat{h}_2\Delta t/\hbar} e^{-i\hat{h}_1\Delta t/2\hbar}, \tag{5.23}$$

which, as in the split-operator case, leads to half-time steps at the beginning and at the end of the time evolution.

Examples

A: Transverse Field Ising Model

For the case of the TFIM, we split the Hamiltonian into

$$\hat{H} = \underbrace{\sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z}_{\hat{h}_1} \; - \; \underbrace{\sum_i h_i \sigma_i^x}_{\hat{h}_2} . \tag{5.24}$$

Both $\hat{h}_1$ and $\hat{h}_2$ can be explicitly exponentiated. First, the Ising term $\hat{h}_1$ is diagonal in the z basis and can be written as

$$e^{-i\hat{h}_1 \Delta t/\hbar} = \prod_{\langle ij \rangle} e^{-i\Delta t J_{ij} s_i^z s_j^z/\hbar}, \tag{5.25}$$

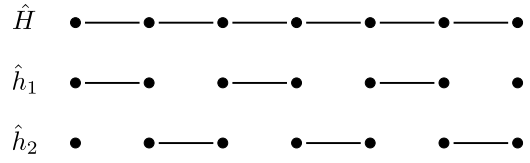
where s_i^z is the eigenvalue of σ_i^z. The local field in $\hat{h}_2$, on the other hand, is not diagonal, but can be exponentiated for each site individually,

$$e^{i\Delta t h_i \sigma^x/\hbar} = \begin{pmatrix} \cos(\Delta t h_i/\hbar) & i\sin(\Delta t h_i/\hbar) \\ i\sin(\Delta t h_i/\hbar) & \cos(\Delta t h_i/\hbar) \end{pmatrix}. \tag{5.26}$$

Note that, as in the case of exact diagonalization, both terms $\hat{h}_1$ and $\hat{h}_2$ can be either written as a direct product or calculated on the fly given a state in the z basis; we never have to store the full evolution operator.

B: XXZ model

For the XXZ model—and thus, the Heisenberg model—we split the interaction bonds into disjoint sets



$$\hat{H} = \hat{h}_1 + \hat{h}_2 = \hat{H}_{\text{even}} + \hat{H}_{\text{odd}} \tag{5.27}$$

with

$$\begin{aligned} \hat{H}_{\text{even}} &= J \sum_i \left[\frac{1}{2} \left(\hat{S}_{2i}^+ \hat{S}_{2i+1}^- + \hat{S}_{2i}^- \hat{S}_{2i+1}^+ \right) + \Delta \hat{S}_{2i}^z \hat{S}_{2i+1}^z \right], \\ \hat{H}_{\text{odd}} &= J \sum_i \left[\frac{1}{2} \left(\hat{S}_{2i-1}^+ \hat{S}_{2i}^- + \hat{S}_{2i-1}^- \hat{S}_{2i}^+ \right) + \Delta \hat{S}_{2i-1}^z \hat{S}_{2i}^z \right]. \end{aligned} \tag{5.28}$$

Both $\hat{H}_{\text{even}}$ and $\hat{H}_{\text{odd}}$ contain only mutually commuting terms that we can individually exponentiate, yielding for two neighboring sites

$$\exp\left(i\Delta t \, \Delta \frac{J}{4} \right) \begin{pmatrix} e^{-i\Delta t \, \Delta \frac{J}{2}} & 0 & 0 & 0 \\ 0 & \cos(\Delta t J/2) & -i\sin(\Delta t J/2) & 0 \\ 0 & -i\sin(\Delta t J/2) & \cos(\Delta t J/2) & 0 \\ 0 & 0 & 0 & e^{-i\Delta t \, \Delta \frac{J}{2}} \end{pmatrix}. \tag{5.29}$$

Imaginary-time evolution

We can use the time-evolution protocol discussed above to obtain the ground state by replacing

$$it \to \tau. \tag{5.30}$$

The *imaginary-time evolution* reads

$$|\psi(\tau)\rangle = e^{-\tau \hat{H}} |\psi(0)\rangle . \tag{5.31}$$

Note an important difference with respect to the real (or physical) time evolution: in the imaginary-time case, the evolution is no longer unitary, it will change the norm of the initial state. However, we can use imaginary-time evolution as an alternative scheme to find the ground state of a given Hamiltonian $\hat{H}$.

To see this, we start from a random state $|\psi_0\rangle = \sum_i c_i |i\rangle$, where $\hat{H} |i\rangle = E_i |i\rangle$. Then,

$$e^{-\tau \hat{H}} |\psi(0)\rangle = \sum_i c_i e^{-E_i \tau} |i\rangle = e^{-E_0 \tau} \left[c_0 |0\rangle + \sum_{k>0} e^{-\Delta E_k \tau} c_k |k\rangle \right], \tag{5.32}$$

where $\Delta E_k = E_k - E_0 \geq 0$. Thus, provided that the initial state has not been chosen orthogonal to the exact ground state, i.e. $|c_0| \neq 0$, the imaginary-time evolution converges to the exact ground state by suppressing the amplitudes of excited states exponentially fast in the product $\Delta E_k \tau$.