# Chapter 1 <br> Introduction to quantum plasma simulations 

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#### Abstract

This chapter contains a brief introduction to the field of quantum simulations. Beginning with a numerical treatment of single-particle problems by exact numerical solution of the time-dependent Schrödinger equation, we demonstrate concepts useful in the computational treatment of quantum systems. These rather basic techniques are limited by the number of particles, $N$. Considering an increase of system size, approximation methods arising from many-particle theories are necessary. Here, we introduce two powerful approaches: the (time-dependent) Hartree-Fock method with improvements for inclusion of correlations based on nonequilibrium Green's functions and, for the calculation of time-independent phenomena, a rigorous quantum Monte Carlo technique. These computational tools complement each other and thus provide for a comprehensive theoretical modelling of quantum plasmas.


### 1.1 Introduction

Modern experimental techniques allow for the selective manipulation of small microand nanoscale systems (quantum plasmas) of even less than one hundred particles. Although the fundamental physical laws which govern these measurements are wellknown, exact analytical solutions are available only for a very limited number of many-particle systems, such as ideal solids (i.e. highly periodic structures without any lattice defects or distortions) or non-interacting classical (i.e. $\Gamma \ll 1$ ) or quantum gases ( $r_{\mathrm{s}} \ll 1$ ). Consideration of interaction makes things much more interesting, but also more complex and theoretically challenging. In most practical cases the fundamental many-body Hamiltonian, Eq. (1.1), cannot be directly diagonalized and more efficient numerical methods are needed. In fact, even simple models used to

[^0]describe interacting quantum systems in the regime of strong particle correlations are computationally very demanding (see the chapter by Bonitz et al.).

In the investigation of ground states and phase transitions, we utilize different classical and quantum bottom-up approaches. This means that the theoretical description starts at the microscopic level of individual particles and, thereby, takes full account of all microscopic many-particle interactions. The only simulation input data involved are the fundamental pair interaction potentials as well as the boundary (confinement) conditions. Hence, the theoretical framework of computational bottom-up methods on hand allows for highly flexible modeling with regard to the specific experimental setup (trap geometry, external fields, number of particles etc.) and yields direct results that are free from any fitting parameters.

The numerical modelling of quantum systems starts from the fundamental manybody Hamiltonian introduced in the previous chapter,

$$
\begin{equation*}
\hat{H}=\sum_{i=1}^{N} \frac{\hat{P}_{i}^{2}}{2 m_{i}}+\sum_{i=1}^{N} V_{i}\left(\boldsymbol{r}_{i}, t\right)+\frac{1}{2} \sum_{i \neq j}^{N} w\left(\boldsymbol{r}_{i}, \boldsymbol{r}_{j}\right) . \tag{1.1}
\end{equation*}
$$

Again, $N$ is the particle number involved, $m_{i}$ the mass of the $i^{\text {th }}$ particle, $V_{i}\left(\boldsymbol{r}_{i}, t\right)$ the single-particle potential (e.g. external confinement, time-dependent perturbations, $\ldots$ ) of the $i^{\text {th }}$ particle and $w\left(\boldsymbol{r}_{i}, \boldsymbol{r}_{j}\right)$ the binary interaction between the $i^{\text {th }}$ and $j^{\text {th }}$ particles, e.g. the Coulomb interaction between charged particles $w\left(\boldsymbol{r}_{i}, \boldsymbol{r}_{j}\right)=$ $e^{2} /\left|\boldsymbol{r}_{i}-\boldsymbol{r}_{j}\right|$.

The Hamiltonian, Eq. (1.1), fully describes the system of interest, its ground state (equilibrium) properties as well as its dynamical behavior following a perturbation, $V(t)$. The first part of this introduction deals with solution schemes for investigation of the temporal development of excited systems on the basis of the single-particle time-dependent Schrödinger equation (TDSE), section 1.2. Then, in section 1.3, we discuss equilibrium and non-equilibrium properties of many-body systems by means of (time-dependent) Hartree-Fock (HF, TDHF) simulations and systematic improvement of the approximation with respect to the binary inter-particle interaction $w$. The chapter continues with an overview of the path integral Monte Carlo (PIMC) method, which allows for a finite temperature description of equilibrium properties of large quantum systems in section 1.4.

### 1.2 Time-dependent Schrödinger equation

Time-dependent phenomena, such as ionization, scattering and excitation, are accurately described within the framework of the time-dependent Schrödinger equation, which reads as

$$
\begin{equation*}
\mathrm{i} \hbar \frac{\partial}{\partial t} \Psi\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{N}, t\right)=\hat{H} \Psi\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{N}, t\right) \tag{1.2}
\end{equation*}
$$

$\boldsymbol{x}_{i}=\left(\boldsymbol{r}_{i}, \sigma_{i}\right)$ denotes the combination of the spatial coordinate vector, $\boldsymbol{r}_{i}$, and the spin variable $\sigma_{i}$.

Due to the great complexity of the time-dependent problem, the many-body TDSE, Eq. (1.2), can only be solved in very few cases. Therefore, the following discussion of the numerical treatment involves two parts: the exact solution of the one-particle $(N=1)$ TDSE and the approximative solution of the many-body $(N>1)$ TDSE in the next section, see section 1.3.

In the atomic system of units, with $\hbar=m=e=1$, Eq. (1.2) for one particle simplifies to

$$
\begin{equation*}
\mathrm{i} \frac{\partial}{\partial t} \Psi(\boldsymbol{r}, t)=-\frac{1}{2} \Delta \Psi(\boldsymbol{r}, t)+V(\boldsymbol{r}, t) \Psi(\boldsymbol{r}, t) \tag{1.3}
\end{equation*}
$$

where the spin degree of freedom is neglected. The numerical solution of the TDSE is a widely studied subject. There exist many different approaches. Each computational technique has its own range of applicability and one has to choose carefully the most suitable investigative procedure as this can enormously affect the resulting efficiency and accuracy.

The formal solution of the TDSE for slow time variation of $V(\boldsymbol{r}, t)$ is given by the time evolution operator

$$
\begin{equation*}
\hat{U}\left(t, t_{0}\right)=\exp \left[-i \hat{H}\left(t-t_{0}\right)\right] \Psi_{0}(\boldsymbol{r}) \tag{1.4}
\end{equation*}
$$

where the corresponding time evolution of the wavefunction $\Psi(\boldsymbol{r}, t)$ takes the form

$$
\begin{equation*}
\Psi(\boldsymbol{r}, t)=\hat{U}\left(t, t_{0}\right) \Psi_{0}(\boldsymbol{r}) \tag{1.5}
\end{equation*}
$$

Here, $\Psi_{0}(\boldsymbol{r})=\Psi\left(\boldsymbol{r}, t \equiv t_{0}\right)$ denotes the initial condition initial condition, that is, the state of the system at initial time $t_{0}$ of the time evolution. Since we are, for numerical reasons, interested in propagation over a small time step of duration $\Delta t$, we only consider the case of Hamilton operators which are not explicitly time-dependent. The external potential, $\hat{V}(\mathbf{r}, t)$, is taken to be slowly time-dependent, e.g., by modelling an external perturbation (laser field, etc.). Otherwise, $\hat{U}$ would take a more complicated form, which is well-known from text-book quantum mechanics. Here, the main idea is, that $\hat{V}(\boldsymbol{r}, t)$ is approximated to be constant during a certain, small time interval $\Delta t$. This can (always) be assured by the choice of a sufficiently small $\Delta t$. In the following we will discuss two methods to solve Eq. (1.5) numerically, which have advantages for different types of systems.

### 1.2.1 1D-Crank-Nicolson method

In this tutorial, we concentrate on the solution of the one-dimensional form of Eq. (1.3), which reads as

$$
\begin{equation*}
\mathrm{i} \frac{\partial}{\partial t} \Psi(x, t)=-\frac{1}{2} \frac{\mathrm{~d}^{2}}{\mathrm{~d} x^{2}} \Psi(x, t)+V(x, t) \Psi(x, t) \tag{1.6}
\end{equation*}
$$

The generalization of the described method to systems of higher dimensions (e.g. by operator splitting) can be found in the literature, e.g. [1]. Eq. (1.6) is a complex diffusion-like initial value problem which has to be supplemented by boundary conditions.

A stable, implicit time evolution scheme, which leads to the Crank-Nicolson procedure is based on Cayley's form of the time evolution operator $\mathrm{e}^{-i \hat{H} \Delta t}$ [1], which is the lowest order of a Padé expansion of the exponential function,

$$
\begin{equation*}
\mathrm{e}^{-i \hat{H} t} \approx \frac{1-\frac{1}{2} \mathrm{i} \hat{H} \Delta t}{1+\frac{1}{2} \mathrm{i} \hat{H} \Delta t} \tag{1.7}
\end{equation*}
$$

This expansion implies a unitary time evolution, hence the normalization of the wave function,

$$
\begin{equation*}
n(x, t)=\int_{-\infty}^{\infty}|\Psi(x, t)|^{2} \mathrm{~d} x \tag{1.8}
\end{equation*}
$$

is assured to be one for all times $t$, which one might easily show for our case by inserting Eq. (1.7) into Eq. (1.8). In contrast to explicit schemes, where the TDSE is solved for the wave function $\Psi$ and then integrated with respect to $t$, implicit schemes are numerically more advanced. Generally, in such an implicit scheme, the wave function is not directly accessable, but has to be obtained by solving a system of linear equations.

Further, we discretize our spatial coordinate $x$ by introducing a spacing $\Delta x$, cf. figure 1.1. Therefore, for $x \in\left[x_{i}, \ldots, x_{i+1}\right]$ with $\Delta x=\left|x_{i+1}-x_{i}\right|$ we write $\Psi_{i}^{n} \equiv \Psi(x, t)$. The index $i=1 \ldots N_{x}$ indicates the spatial discretization with the step size $\Delta x$, whereas the superscript $n$ denotes the corresponding discretization in time. Hence, $n+1 \equiv t+\Delta t$ and $i+1 \equiv x+\Delta x$, for example.

Using Eq. (1.7) as an approximation for $\hat{U}$ in Eq. (1.5), one represents the propagation of $\Psi_{i}^{n}$ to the state $\Psi_{i}^{n+1}$ of later time as

$$
\begin{equation*}
\left(1+\frac{1}{2} \mathrm{i} \hat{H} \Delta t\right) \Psi_{i}^{n+1}=\left(1-\frac{1}{2} \mathrm{i} \hat{H} \Delta t\right) \Psi_{i}^{n} \tag{1.9}
\end{equation*}
$$

Now, the remaining task is to find a representation of the Hamilton operator $\hat{H}$. In our case, it is replaced by a finite difference approximation. We consider a second-order expression for the derivatives,

$$
\begin{equation*}
\frac{\mathrm{d}^{2}}{\mathrm{~d} x^{2}} \Psi(x, t) \approx \frac{\Psi_{i+1}^{n}-2 \Psi_{i}^{n}+\Psi_{i-1}^{n}}{(\Delta x)^{2}} \tag{1.10}
\end{equation*}
$$



Fig. 1.1 Schematic view of the one-dimensional grid. The TDSE is solved within the marked region on a number $N_{x}$ discrete grid points. $i=1$ and $i=N_{x}$ are defined by the boundary conditions.

Of course, higher-order schemes can be implemented; for a recent adaption of the methods see e.g. [2].

Combining Eqs. (1.9) and (1.10) with $\alpha=i \Delta t /(2 \Delta x)^{2}$ and

$$
\begin{equation*}
a_{i}=-\alpha=c_{i}, \quad b_{i}=1+2 \alpha+\frac{1}{2} i \Delta t V_{i}^{n+1}, \quad i=2 \ldots N_{x}-1 \tag{1.11}
\end{equation*}
$$

the l.h.s. of Eq. (1.9) is given by

$$
\begin{equation*}
\left(1+\frac{1}{2} i \Delta t \hat{H}\right) \Psi_{i}^{n+1}=a_{i} \Psi_{i-1}^{n+1}+b_{i} \Psi_{i}^{n+1}+c_{i} \Psi_{i+1}^{n+1} . \tag{1.12}
\end{equation*}
$$

Analogously, the r.h.s. of Eq. (1.9) transforms into

$$
\begin{equation*}
\left(1-\frac{1}{2} \mathrm{i} \hat{H} \Delta t\right) \Psi_{i}^{n}=\Psi_{i}^{n}\left(1-2 \alpha-\frac{1}{2} i \Delta t V_{i}^{n}\right)+\alpha \Psi_{i-1}^{n}+\alpha \Psi_{i+1}^{n} \equiv r_{i}^{n} \tag{1.13}
\end{equation*}
$$

Expressing the combination of Eq. (1.12) and Eq. (1.13) in matrix form one finds a tridiagonal form of the system of linear equations for the $N_{x}$ unknown variables $\Psi_{i}^{n+1}, i=1 \ldots N_{x}$ :

$$
\left(\begin{array}{cccc}
b_{1} & c_{1} & 0 & 0  \tag{1.14}\\
a_{2} & b_{2} & c_{2} & 0 \\
\cdot & \cdot & \cdot & \cdot \\
0 & 0 & a_{N_{x}} & b_{N_{x}}
\end{array}\right) \cdot\left(\begin{array}{c}
\Psi_{1}^{n+1} \\
\Psi_{2}^{n+1} \\
\cdot \\
\Psi_{N_{x}}^{n+1}
\end{array}\right)=\left(\begin{array}{c}
r_{1}^{n} \\
r_{2}^{n} \\
\cdot \\
r_{N_{x}}^{n}
\end{array}\right)
$$

The elements $b_{1}, c_{1}$ and $r_{1}^{n}$ are defined by the boundary conditions at the left edge of the grid (an example is given below). Similarly, $b_{N_{x}}, c_{N_{x}}$ and $r_{N_{x}}^{n}$ are defined at the right edge. Since the matrix of coefficients in Eq. (1.14) is very sparse, it can be solved and stored very efficiently. Many numerical libraries have specialized routines implemented to handle such matrices.

### 1.2.1.1 Boundary conditions

The initial value problem of the TDSE is supplemented by boundary conditions, which close the partial differential equation mathematically. Several possibilities are available, e.g. Dirichlet, von Neumann and absorbing conditions. They are chosen by physical observations and define the system of interest. In this introduction only the first one (Dirichlet) is considered.

In this case, the wave function is taken to vanish at the boundaries of the system,

$$
\begin{equation*}
\lim _{x \rightarrow \infty} \Psi(x, t) \rightarrow 0 \quad \text { and } \quad \lim _{x \rightarrow-\infty} \Psi(x, t) \rightarrow 0 \tag{1.15}
\end{equation*}
$$

and a simulation box with reflecting grid boundaries is created. This special type of Dirichlet boundary conditions assures conservation of the normalization of $\Psi$ for all times if no dissipation is artificially included (e.g. by an absorbing potential, see
below). Eq. (1.15) can be fulfilled if the wave function is zero at the right-most and the left-most element on the grid, i.e. $\Psi_{0}^{n}=\Psi_{N_{x}}^{n}=0$ for all time steps $n$. This can be satisfied by modifying the first and the last elements in the tridiagonal system of equations, Eq. (1.14). As an exercise, the reader is left with the calculation, that gives $a_{1, N_{x}}=c_{1, N_{x}}=r_{1, N_{x}}=0$ and $b_{1, N_{x}}=1+i$. Obviously, this type of boundary condition requires large spatial grids in order to allow for long simulation runs without influence of reflected parts of the wave function stemming from non-physical reflection of $\Psi$ at the end of the simulation box.

### 1.2.1.2 Absorbing boundary conditions



Fig. 1.2 Influence of a linear imaginary absorbing potential $i V(x)$ : Absorption of a 1D wave packet [ $k=2.0$ a.u., Eq. (1.20)]. Almost the whole packet is absorbed and only a fraction smaller than $10^{-7}$ is reflected, see inset for normalization of $\Psi$. All quantities are given in atomic units (a.u.).

A technique of avoiding computationally expensive large grids is the introduction of absorbing boundary conditions. In fact, there are basically two methods to be found in the literature. The first one is especially important for one-dimensional calculations. It is based on a mathematical theory which allows complete absorption of the wave function at a specific grid point [3]. Its computational implementation is difficult and for higher-dimensional systems it is not applicable [4]. We will describe a simpler, easy to implement approach, which uses additional potentials in the system but lacks of mathematical rigor.

If a spatially confined imaginary part is added to the one-particle potential $V(x, t)$, the wave function $\Psi(x, t)$ is damped during the time of propagation over this region. This can be rationalized in terms of the equation of continuity since this so-called optical potential acts like a dissipation term. One finds that this damping effect increases with higher energies of the propagated particle. Thus, the faster a particle
moves the more efficiently it can be absorbed by the potential. It should be mentioned that such absorbing potentials have to be chosen carefully. Every change in the potential, no matter if real or imaginary, leads to a reflected part of the wave function. Roughly speaking, the smoother the spatial variation of the imaginary potential, the better it will work. The simplest conceptual version is, for example, given by a linear potential. More efficient potentials are available in the literature [5, 6].

Fig. 1.2 shows the absorption of a one-dimensional wave packet for such a linear, imaginary potential, indicated by the black line. Only a very small fraction $\left(10^{-7}\right)$ survives the damping and is reflected. Such grid boundaries are of course not boundary conditions in a mathematical sense. The system of equations, Eq. (1.14), has yet to be closed by Dirichlet conditions discussed above.

### 1.2.1.3 Initial conditions

Finally, the time propagation of the TDSE needs an initial condition, $\Psi_{0}(x)=$ $\Psi\left(x, t=t_{0}\right)$. The choice of this state reflects the physical motivation of the problem. In the following, we will discuss two possibilities: (i) the construction of eigenstates and (ii) the treatment of free particles by Gaussian wave packets .
(i) Imaginary Time Propagation (ITP). The above described time propagation code can easily be used to calculate stationary states by replacing the time $t$ by an imaginary time it [4], which transforms the TDSE into a diffusion equation. An arbitrary state can be written as a superposition of eigenstates with expansion coefficient $c_{j}=\left\langle\psi_{j} \mid \Psi(t)\right\rangle$,

$$
\begin{equation*}
|\Psi(t)\rangle=\sum_{j} c_{j} \exp \left(-\mathrm{i} E_{j} t\right)\left|\psi_{j}\right\rangle \tag{1.16}
\end{equation*}
$$

with $\left|\psi_{j}\right\rangle$ describing the stationary states. Now, if the imaginary time is inserted, one obtains

$$
\begin{equation*}
|\Psi(t)\rangle=\sum_{j} c_{j} \exp \left(E_{j} t\right)\left|\psi_{j}\right\rangle \tag{1.17}
\end{equation*}
$$

and the corresponding states are exponentially decaying or increasing during the TDSE propagation depending on the sign of the energy eigenvalue $E_{j}$. Only the ground state survives because it decays less or increases much faster than the other states. Of course this scheme does not conserve the normalization of the $\Psi$. Therefore, the wave function has to be renormalized at each time step.

Excited states, $(n+1)$, where $n$ denotes the highest, previously constructed state, are also accessable by this procedure: The Schmidt orthogonalization of $|\psi(t)\rangle$

$$
\begin{equation*}
\psi_{n+1}^{\perp}(\boldsymbol{r})=\psi_{n+1}(\boldsymbol{r})-\sum_{i=0}^{n}\left(\int_{-\infty}^{\infty} \mathrm{d}^{3} \boldsymbol{r} \psi_{n+1}^{*}(\boldsymbol{r}) \psi_{i}(\boldsymbol{r})\right) \cdot \psi_{i}(\boldsymbol{r}) \tag{1.18}
\end{equation*}
$$

at each time step will force the wave function to converge to the next unknown eigenfunction. The initial wave function for the ITP may be chosen to be completely
random or, what is better for convergence reasons, as near to the ground (excited) state wave function as possible.

During the imaginary iteration procedure several convergence indicators can be used. The total energy appears to be an improper criterion especially for higher excited states. Its convergence is very fast but not sensitive to density changes. Thus a density based quantity such as

$$
\begin{equation*}
\Delta \xi=\int_{-\infty}^{\infty}|\Psi(x, t)-\Psi(x, t+\Delta t)|^{2} \mathrm{~d} x \tag{1.19}
\end{equation*}
$$

is found to be of higher accuracy. The ITP method is, in contrast to other methods like the shooting algorithm [7], applicable to arbitrary potentials in an arbitrary number of spatial dimensions. It may be understood as a powerful method for the diagonalization of $\hat{H}$ in the spatial coordinate basis representation.

Gaussian wave packets . For other interesting physical questions, i.e. scattering situations, it may be of interest, to model initially free electrons. One possibility is the usage of Gaussian wave packets, see e.g. [8]:

$$
\begin{equation*}
\Psi\left(x, t_{0}\right)=\frac{1}{\sqrt{2 \pi \sigma}} \exp \left(-\frac{\left(x-x_{0}\right)^{2}}{2 \sigma^{2}}\right) \exp \left(\mathrm{i} k_{0} x\right) \tag{1.20}
\end{equation*}
$$

The initial momentum $k_{0}$ describes how fast the electron travels, whereas $x_{0}$ determines its initial position at time $t=t_{0}$ and $\sigma$ its spatial spreading. Through Heisenberg's uncertainty law, $\sigma$ also defines the momentum distribution, which corresponds to a smoothed energy distribution via the free particle dispersion law $E=k_{0}^{2} / 2$. All these issues have to be kept in mind in order to make accurate simulations of quantum systems.

### 1.2.2 TDSE solution in basis representation

In this section, we describe a different solution scheme for the one-particle TDSE, cf. Eq. (1.3), which only relies on matrix multiplications and (at least one) diagonalization of the Hamilton matrix . Depending on the systems considered (e.g. confined systems), it is very efficient. The applied techniques described here are the basis for the following introduction to Hartree-Fock methods (section 1.3); hence, study of this section is strongly suggested before continuing to the next part.

To start, we express the wave function $|\Psi(t)\rangle$ in a complete orthonormal basis set $\left\{\varphi_{i}\right\}_{i=1 . . \infty}$, where $\left\langle\varphi_{i} \mid \varphi_{j}\right\rangle=\delta_{i j}$ holds:

$$
\begin{equation*}
|\Psi(t)\rangle=\sum_{i=0}^{\infty} c_{i}(t)\left|\varphi_{i}\right\rangle \tag{1.21}
\end{equation*}
$$

The expansion coefficients are given by $c_{i}(t)=\left\langle\varphi_{i} \mid \Psi(t)\right\rangle$. For numerical reasons it is necessary, analogously to the introduction of the finite spatial grid in the previous
section, to truncate the sum in Eq. (1.21) at a finite number $N_{b}$. With this, the basis is no longer complete in the mathematical sense and one has to assure that the chosen basis functions reflect the final solutions as closely as possible, minimizing the required number of basis functions, $N_{b}$. This is a challenging task, especially in the case of highly dynamical behavior of the system considered. During the time evolution, many intermediate states may be accessed and all these states have to be described as accurately as possible by the basis.

As described above, in addition to the Hamilton operator and the corresponding time evolution operator, an initial condition $\Psi\left(t=t_{0}\right)$ is needed, which corresponds to an initial set of expansion coefficients $\left\{c_{i}\left(t_{0}\right)\right\}_{i=1 . . N b}$.

### 1.2.2.1 Deriving a time evolution scheme

The determination of an expression for the time evolution of the vector of $N_{b}$ coefficients $\boldsymbol{c}(t)$ can be achieved by applying the time evolution operator $\hat{U}$ to the initial state: $|\Psi(t)\rangle=\hat{U}\left|\psi_{0}\right\rangle$. To extract $c_{i}(t)$, we expand $|\Psi(t)\rangle$ and insert $\hat{1}=\sum_{i}^{N b}\left|\varphi_{i}\right\rangle\left\langle\varphi_{i}\right|:$

$$
\begin{equation*}
|\Psi(t)\rangle=\sum_{j=0}^{N b} c_{j}(t)\left|\varphi_{j}\right\rangle=\sum_{i}^{N b} \hat{U}\left|\varphi_{i}\right\rangle\left\langle\varphi_{i}\right| \sum_{l}^{N b} c_{l}\left(t=t_{0}\right)\left|\varphi_{l}\right\rangle \tag{1.22}
\end{equation*}
$$

Multiplying the whole equation from the left with $\left\langle\varphi_{k}\right|$ yields

$$
\begin{equation*}
\sum_{j=0}^{N b} c_{j}(t)\left\langle\varphi_{k} \mid \varphi_{j}\right\rangle=\sum_{i=0}^{N b}\left\langle\varphi_{k}\right| \hat{U}\left|\varphi_{i}\right\rangle\left\langle\varphi_{i}\right| \sum_{l=0}^{N b} c_{l}\left(t=t_{0}\right)\left|\varphi_{l}\right\rangle \tag{1.23}
\end{equation*}
$$

Therefore, we finally obtain the time-dependent coefficients as

$$
\begin{equation*}
c_{k}(t)=\sum_{i=0}^{N b} U_{k i} \sum_{l=0}^{N b} c_{l}\left(t=t_{0}\right)\left\langle\varphi_{i} \mid \varphi_{l}\right\rangle=\sum_{i} U_{k i} c_{i}\left(t=t_{0}\right) \tag{1.24}
\end{equation*}
$$

This is simply a matrix product and can be written in the form

$$
\begin{equation*}
\mathbf{c}(t)=\mathbf{U} \cdot \mathbf{c}\left(t=t_{0}\right) \tag{1.25}
\end{equation*}
$$

with $\mathbf{U}=\left\{U_{i j}\right\}_{i, j \in\left\{1, \ldots, N_{b}\right\}}$ denoting an $N_{b} \times N_{b}$ matrix.

### 1.2.2.2 Computation of matrix elements of $\boldsymbol{U}_{i j}$

The remaining problem is to find the basis representation of the time evolution operator $\hat{U}=\exp (\mathrm{i} \hat{H} \Delta t)$, cf. Eq. (1.5), i.e. the $\left(N_{b}\right)^{2}$ complex matrix elements $U_{i j}$ of $\mathbf{U}$.

Applying basic linear algebra leads to

$$
\begin{equation*}
U_{i j}=\left\langle\varphi_{i}\right| \hat{U}\left|\varphi_{j}\right\rangle=\sum_{k=0}^{\infty}\left\langle\varphi_{i} \mid \psi_{k}\right\rangle\left\langle\psi_{k} \mid \varphi_{j}\right\rangle \exp \left(\mathrm{i} E_{k} \Delta t\right) \tag{1.26}
\end{equation*}
$$

Here, $\left|\psi_{k}\right\rangle$ are the eigenfunctions of $\hat{H}$ corresponding to the eigenvalue $E_{m}$. The first two factors on the right-hand-side of Eq. (1.26) are simply the eigenvectors of $\hat{H}$ in the basis representation $\left|\varphi_{i}\right\rangle_{i=1 . . N b}$, which can be obtained by a diagonalization of the Hamiltonian. This diagonalization of $\hat{H}$ has to be performed for each temporal change in $\hat{H}$ which leads to a computationally very efficient propagation scheme for given excitations. From the obtained (time-dependent) expansion coefficients $c_{i}(t)$, all expectation values can be computed.

Boundary conditions, as considered above, are not to be specified explicitly. They are embedded in the behavior of the chosen basis functions. For the initial moment of time propagation, one only has to specify a certain set of $c_{i}\left(t=t_{0}\right)$, hence it is very easy to prepare a system in a bound state if the basis is chosen to be a set of associated eigenstates. Thus it is clear, that this method has advantages for localized systems in traps, atoms, etc., but may reach its limits in the consideration of situations where combinations of free particles and localized states are involved. For this case, grid methods perform better.

### 1.2.3 Computational example: electron scattering in a laser field

In this section, we demonstrate the utility of the above-described algorithms by their application to a simple physical system, which is, due to its computational complexity, analytically not accessable. Let us consider a free electron, represented by a wave packet of Gaussian shape , cf. Eq. (1.20), travelling with a momentum $k_{0}$ towards an ion. The whole system is radiated with a strong, linearly polarized laser field, modelled by the potential (in dipole approximation)

$$
\begin{equation*}
V_{\text {laser }}(x, t)=-E_{0} x \cos (\omega t) . \tag{1.27}
\end{equation*}
$$

The electron may now absorb energy from the laser field during the scattering process, and due to the quantization character, only in amounts equal to $\omega$ (remember: $\hbar=m=e=1$ in our system of units). The setup of the system is schematically drawn in fig. 1.3.

After propagating the TDSE with the Crank-Nicolson procedure described above, the resulting wave function outside the ion-potential is transformed by a fast Fourier transform into momentum space. Using the free-particle dispersion relation, $E=p^{2} / 2 m$, the energy distribution is calculated. Fig. 1.4 shows the result of the simulation of such a scattering process with $k_{0}=4.0 \mathrm{a} . \mathrm{u}$. in a strong laser field with parameters given in the figure caption. The sign of the energy indicates forward ( + ) and backward ( - ) scattering, respectively. One easily identifies the peak


Fig. 1.3 Schematic view of the Coulomb scattering process. The electronic wave packet is launched at a distance $x_{0}$ from the ion with a momentum $k_{0}$ directed towards the ion. The whole setup is placed in a strong linearly polarized laser field.
of elastically forward scattered electrons with an energy of $E=k_{0}^{2} / 2=8.0 \mathrm{a} . \mathrm{u}$. In backward direction (negative energies) a large plateau in the energy distribution is formed with two significant cut-off energies, which can easily be obtained using a simple classical theory $[8,9]$. A closer look at the energy spectrum reveals a peak-like structure, where each individual peak is separated by the photon energy $\omega$.


Fig. 1.4 Energy distribution (left) and initial+final electron density (right) of a Coulomb scattering process with $k_{0}=4.0 \mathrm{a} . \mathrm{u}$. in a strong laser field with $\omega=0.2$ a.u., $E_{0}=0.2$ a.u.. Negative (positive) energies indicate backward (forward) scattering.

### 1.3 Hartree-Fock Method

The time-dependent Hartree-Fock (TDHF) method aims at approximately solving the time-dependent $N$-particle Schrödinger equation

$$
\begin{equation*}
-i \frac{\partial}{\partial t} \Psi\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{N}, t\right)=\hat{H} \Psi\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{N}, t\right) \tag{1.28}
\end{equation*}
$$

with $\boldsymbol{x}_{i}=\left(\boldsymbol{r}_{i}, \sigma_{i}\right)$ and Hamiltonian ${ }^{1}$

$$
\begin{equation*}
\hat{H}=\sum_{i=1}^{N}\left(-\frac{\nabla_{\boldsymbol{r}_{i}}^{2}}{2 m}+\sum_{i=1}^{N} V\left(\boldsymbol{r}_{i}, t\right)\right)+\sum_{i<j}^{N} w\left(\boldsymbol{r}_{i}-\boldsymbol{r}_{j}\right) . \tag{1.29}
\end{equation*}
$$

Thereby, it offers partial information when the exact solution is not accessible, e.g. by the numerical techniques described in the last section. The TDHF scheme can be derived from several different (but equivalent) aspects of many-body theory [10]. Here, we concentrate on two common approaches. The first outlines the standard derivation which handles the problem on the level of an approximate $N$-particle wave function, $\Psi\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{N}, t\right)$. The main quantity of the second is based on a two-time generalization of the one-particle density matrix, $\varrho(\boldsymbol{x}, \overline{\boldsymbol{x}} ; t)$-the nonequilibrium Green's function (NEGF) .

The idea of TDHF dates back to Dirac[11] and has had first applications in nuclear collisions and atomic physics [12]. More recent approaches-to name only a few-include the dynamics of electrons in molecules [13], atoms exposed to strong laser fields [14] as well as single and double ionization processes, see e.g. [15] and references therein. Further more, in condensed matter physics and non-ideal plasmas, the TDHF ansatz has been used successfully in the framework of NEGFs [16, 17, 18, 19, 20]. Moreover, the method is closely related to the random phase approximation (RPA) , e.g. as applied in the theory of dielectric functions [21].

Standard approach. Considering fermions, the TDHF method starts with the timedependent Schrödinger equation (1.28) approximating the total many-body wave function to be a totally anti-symmetrized product of one-particle orbitals $\phi_{i}\left(\boldsymbol{x}_{i}, t\right)$ ( $i \in\{1, \ldots, N\}$ ) which depend on time [10]. Thus, $\Psi\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{N}, t\right)$ becomes a single Slater determinant $\mathcal{D}$ according to

$$
\begin{align*}
\Psi\left(\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{N}, t\right) & =\hat{A} \prod_{i=1}^{N} \phi_{i}\left(\boldsymbol{x}_{i}, t\right)=\frac{1}{\sqrt{N!}} \mathcal{D}\left(\phi_{i}\left(\boldsymbol{x}_{j}, t\right)\right)  \tag{1.30}\\
& =:\left|\Psi\left[\phi_{1}, \ldots, \phi_{N}\right]\right\rangle,
\end{align*}
$$

where $\hat{A}$ denotes the anti-symmetrization operator. The equations of motion for the orbitals $\phi_{i}$ then follow from the action functional[15]

$$
\begin{equation*}
A\left[\phi_{1}, \ldots, \phi_{N}\right]=\int_{t_{0}}^{t_{1}} \mathrm{~d} t\left\langle\Psi\left[\phi_{1}, \ldots, \phi_{N}\right]\right| i \frac{\partial}{\partial_{t}}-\hat{H}\left|\Psi\left[\phi_{1}, \ldots, \phi_{N}\right]\right\rangle \tag{1.31}
\end{equation*}
$$

which must be stationary under variations of the orbitals when the constraint $\delta \phi_{i}=0$ $\forall i$ is applied at $t=t_{0}$ and $t=t_{1}$. Using this action principle, the norm of the

[^1]many-body wave function $\Psi$ is conserved while inserting definition (1.30) directly into the TDSE and presuming all $\phi_{i}$ to be orthonormal, i.e. $\left\langle\phi_{i} \mid \phi_{j}\right\rangle=\delta_{i j} \forall t$, leads to a set of equations by which the norm of $\Psi$ varies. The latter approach is more straight forward and leads to the coupled system of equations
\[

$$
\begin{equation*}
i \frac{\partial}{\partial t} \phi_{i}(\boldsymbol{x}, t)=\left(\hat{H}^{0}(\boldsymbol{x}, t)+\hat{\Sigma}[\phi](\boldsymbol{x}, t)\right) \phi_{i}(\boldsymbol{x}, t) \tag{1.32}
\end{equation*}
$$

\]

with the single-particle energy operator $\hat{H}^{0}(\boldsymbol{x}, t)=-\nabla_{\boldsymbol{x}}^{2} /(2 m)+V(\boldsymbol{x}, t)$, and the self-energy operator $\hat{\Sigma}(\boldsymbol{x}, t)$, which accounts for particle-particle interactions. The notation $\Sigma[\phi]$ indicates that the self-energy is a functional of all $\phi_{i}$ with $i=1, \ldots, N$. Further, the sum $\hat{H}^{0}+\hat{\Sigma}$ is often called Fock operator in the literature[14]. Explicitly, the action of the operator $\hat{\Sigma}$ on the orbital $\phi_{i}$ is given by

$$
\begin{align*}
\hat{\Sigma}(\boldsymbol{x}, t) \phi_{i}(\boldsymbol{x}, t)= & \left(\sum_{j} \int \mathrm{~d} \bar{x}\left|\phi_{j}(\overline{\boldsymbol{x}}, t)\right|^{2} w(\boldsymbol{x}-\overline{\boldsymbol{x}})\right) \phi_{i}(\boldsymbol{x}, t) \\
& \left.-\sum_{i<j}^{\prime}\left(\int \mathrm{d} \bar{x}\right] \phi_{i}(\overline{\boldsymbol{x}}, t) \phi_{j}(\overline{\boldsymbol{x}}, t) w(\boldsymbol{x}-\overline{\boldsymbol{x}})\right) \phi_{j}(\boldsymbol{x}, t) \tag{1.33}
\end{align*}
$$

The first term constitutes the classical mean-field (Hartree) potential as an integral over the orbital resolved density $n_{i}(\boldsymbol{x}, t)=\left|\phi_{i}(\boldsymbol{x}, t)\right|^{2}$. The second is the exchange potential (or Fock term) which is the indispensable quantum mechanical correction accounting for anti-symmetrization and the Pauli exclusion principle. In this sense, the ansatz (1.30) neglects any correlation effects which arise from terms of higher than first order in the interaction potential. Systematic improvements of TDHF results are possible, e.g. by multiconfiguration time-dependent Hartree-Fock (MCTDH) theory which involves superpositions of several Slater determinants [22], time-dependent density functional theory (TDDFT) including exchange-correlation functionals [23] or nonequilibrium Green's function theory with higher-order self-energies [24, 16].

Of course, in regard to time evolution, Eq. (1.32) needs to be supplied with initial conditions which are just the stationary (ground state) solutions with $i \partial / \partial_{t} \phi_{i}(\boldsymbol{x}, t)$ replaced by $\epsilon_{i} \phi_{i}^{0}(\boldsymbol{x})$. The energy eigenvalues $\epsilon_{i}$ and the corresponding orbitals $\phi_{i}^{0}(\boldsymbol{x})$ can be computed either by propagation of Eq. (1.32) in imaginary time -as described for the TDSE in the previous section-or by iterating the stationary equations until a self-consistent solution $\left\{\epsilon_{i}, \phi_{i}^{0}(\boldsymbol{x})\right\}$ is obtained (self-consistent field method, see e.g. [25, 26, 27]). However, the latter procedure is, in contrast to the imaginary time propagation technique, not conveniently performed on spatial grids, but it is instead transformed into a generalized eigenvalue problem by using a basis expansion for the initial set of orbitals:

$$
\begin{equation*}
\phi_{i}^{0}(\boldsymbol{x})=\sum_{j=1}^{n_{b}} c_{j i} \varphi_{j}(\boldsymbol{x}), \tag{1.34}
\end{equation*}
$$

where the $n_{b}$ - in principle - arbitrary (or adapted) functions $\varphi_{j}(\boldsymbol{x})$ have overlap $O_{i j}=\left\langle\varphi_{i} \mid \varphi_{j}\right\rangle$, and $c_{j i}$ are the unknown coefficients. Using (1.34) in the stationary
form of Eq. (1.32) and integrating over space yields the so-called Roothaan-Hall equations[27]

$$
\begin{equation*}
\sum_{k=1}^{n_{b}}\left(H_{i k}^{0}+\Sigma_{i k}[c]-\epsilon_{j} O_{i k}\right) c_{k j}=0 \tag{1.35}
\end{equation*}
$$

Here, the one-particle energy and the self-energy become matrices, $\hat{H}^{0}(\boldsymbol{x}) \rightarrow H_{i j}^{0}$ and $\hat{\Sigma}[\phi](\boldsymbol{x}) \rightarrow \Sigma_{i j}[c]$, which are defined by

$$
\begin{align*}
H_{i j}^{0} & =\int \mathrm{d} x \varphi_{i}^{*}(\boldsymbol{x}) \hat{H}^{0}(\boldsymbol{x}) \varphi_{j}(\boldsymbol{x})  \tag{1.36}\\
\Sigma_{i j}[c] & =\sum_{k l}\left(w_{i j, k l}-w_{i l, k j}\right) \varrho_{k l}[c] \tag{1.37}
\end{align*}
$$

with the single-particle density matrix, $\varrho_{i j}[c]=\sum_{k \leq N} c_{i k} c_{j k}^{*}$, and two-particle integrals given by

$$
\begin{equation*}
w_{i j, k l}=\iint \mathrm{d} x \mathrm{~d} \bar{x} \varphi_{i}^{*}(\boldsymbol{x}) \varphi_{k}^{*}(\overline{\boldsymbol{x}}) w(\boldsymbol{x}-\overline{\boldsymbol{x}}) \varphi_{j}(\boldsymbol{x}) \varphi_{l}(\overline{\boldsymbol{x}}) \tag{1.38}
\end{equation*}
$$

To solve the Roothaan-Hall equations iteratively, one starts from a random or trial state characterized by the density matrix $\varrho_{i j}$ [provide either $\varrho_{i j}$ or the expansion coefficients $c_{i j}$ ]. Then, the self-energy is computed from Eq. (1.37) and the general eigenvalue problem (1.35) is solved for a new set of coefficients $c_{i j}$. The procedure is finally repeated until self-consistency is achieved, in which all elements $\varrho_{i j}$ have reached a fixed point. However, the solution contains, in general, more than $N$ orbitals. The $N$ energetically lowest (occupied) orbitals, $\phi_{i \leq N}^{0}$, form the desired (pure) ground state wave function, whereas the remaining $n_{b}-N$ (virtual) orbitals are connected with the excited states of the system. Hence, the self-consistent field method also allows for the description of mixed states when a finite temperature (grand canonical) density matrix, $\varrho_{i j} \rightarrow \sum_{k=1}^{n_{b}} c_{i k} f_{\beta}\left(\epsilon_{k}-\mu\right) c_{j k}^{*}$, is used, where $f_{\beta}\left(\epsilon_{i}-\mu\right)$ denotes the Fermi-Dirac distribution with inverse temperature $\beta=\left(k_{\mathrm{B}} T\right)^{-1}$ and $\mu$ is the chemical potential obtained from $\sum_{k=1}^{n_{b}} f_{\beta}\left(\epsilon_{i}-\mu\right)=N$. However, note that the time-dependent Hartree-Fock equations (1.32) do not provide for the propagation of mixed states.

NEGF approach. The theory of nonequilibrium Green's functions[24, 16] offers an alternative formulation of the TDHF method in terms of a generalized on6e-particle density matrix $G(\boldsymbol{x}, t ; \overline{\boldsymbol{x}}, \bar{t})$, which is called a Green's function and depends on two space-time variables-again $\boldsymbol{x}=(\boldsymbol{r}, \sigma)$. Utilizing NEGFs it is, particularly, possible to go beyond the ansatz (1.30) by systematically including correlations via higherorder self-energy contributions[24, 29]. Also, the approach is capable of handling the time-dependence of mixed states.

Using $\hbar=1$, the nonequilibrium Green's function is defined by

$$
\begin{equation*}
G(\boldsymbol{x}, t ; \overline{\boldsymbol{x}}, \bar{t})=-i\left\langle T_{\mathcal{C}} \hat{\psi}_{H}(\boldsymbol{x}, t) \hat{\psi}_{H}^{\dagger}(\overline{\boldsymbol{x}}, \bar{t})\right\rangle, \quad\langle\ldots\rangle=\operatorname{Tr}\{\varrho \ldots\} \tag{1.39}
\end{equation*}
$$

with fermionic field operators $\hat{\psi}_{H}(\boldsymbol{x}, t)$ in the Heisenberg picture ${ }^{2}$, and timearguments $t$ and $\bar{t}$ defined on the complex Schwinger/Keldysh contour $\mathcal{C}$ [28]. Further, the operator $T_{\mathcal{C}}$ ensures time-ordering on $\mathcal{C}$. From $G$, the one-particle density matrix, and many other observables [18], are recovered in the limit of equal times:

$$
\begin{equation*}
\varrho(\boldsymbol{x}, \overline{\boldsymbol{x}} ; t)=-i G^{<}(\boldsymbol{x}, t ; \overline{\boldsymbol{x}}, t), \tag{1.40}
\end{equation*}
$$

with definition $G(1, \overline{1})=\theta(t-\bar{t}) G^{>}(1, \overline{1})-\theta(\bar{t}-t) G^{<}(1, \overline{1})$ and notation $1=(\boldsymbol{x}, t)$ and $\overline{1}=(\overline{\boldsymbol{x}}, \bar{t})$. The two-time Green's function $G$ obeys generalized kinetic equations , the Keldysh/Kadanoff-Baym equations (KBE) [24]

$$
\begin{align*}
{\left[i \frac{\partial}{\partial t}-\hat{H}^{0}(1)\right] G(1, \overline{1}) } & =\delta_{\mathcal{C}}(1-\overline{1})-\int_{\mathcal{C}} \mathrm{d} 2 \Sigma[G](1,2) G(2, \overline{1})  \tag{1.41a}\\
{\left[-i \frac{\partial}{\partial \bar{t}}-\hat{H}^{0}(\overline{1})\right] G(1, \overline{1}) } & =\delta_{\mathcal{C}}(1-\overline{1})-\int_{\mathcal{C}} \mathrm{d} 2 \Sigma[G](1,2) G(2, \overline{1}) \tag{1.41b}
\end{align*}
$$

with $\delta_{\mathcal{C}}(1-\overline{1})=\delta_{\mathcal{C}}(t-\bar{t}) \delta(\boldsymbol{x}-\overline{\boldsymbol{x}}), \int_{\mathcal{C}} \mathrm{d} 2:=\int \mathrm{d} x_{2} \int_{\mathcal{C}} \mathrm{d} t_{2}$ and self-energy $\Sigma[G]$. The TDHF problem is then formulated via the approximation

$$
\begin{equation*}
\Sigma[G](1, \overline{1})=i \delta(1-\overline{1}) \int_{\mathcal{C}} \mathrm{d} 3 W(1-3) G\left(3,3^{+}\right)-i G(1, \overline{1}) W\left(1^{+}-\overline{1}\right) \tag{1.42}
\end{equation*}
$$

where $W(1-\overline{1})=\delta_{\mathcal{C}}(t-\bar{t}) w(\boldsymbol{x}-\overline{\boldsymbol{x}})$, and $1^{+}$indicates the limit $t \rightarrow t+\varepsilon_{>0}$. The explicit form of Eq. (1.42) is readily obtained from an irreducible diagrammatic expansion of the self-energy [29] retaining only first-order terms in $W$, and has the same structure as Eq. (1.33): The first term is the time-local Hartree potential, the second incorporates exchange features.

The equilibrium solution of the KBE including (1.42) is given by the Matsubara Green's function

$$
\begin{align*}
G^{M}(\boldsymbol{x}, \overline{\boldsymbol{x}} ; \tau) & =\sum_{i, j=1}^{n_{b}} \phi_{i}^{0 *}(\boldsymbol{x}) \phi_{j}^{0}(\boldsymbol{x}) G_{i j}^{M}(\tau),  \tag{1.43}\\
G_{i j}^{M}(\tau) & =\delta_{i j} f_{\beta}\left(\epsilon_{i}-\mu\right) \mathrm{e}^{-\tau\left(\epsilon_{i}-\mu\right)}
\end{align*}
$$

where $\tau \in[-\beta, 0]$. The orbitals $\phi_{i}^{0}$ together with $\epsilon_{i}$ and $\mu$ are solutions of the selfconsistent field method, and any (pure) ground state is obtained in the limit $\beta \rightarrow \infty$. More formally, Eq. (1.43) solves the Dyson equation [the KBE for $t-\bar{t}=i \tau$ ] on the Hartree-Fock level, see e.g. [29, 30] and references therein. Further, $G^{M}(\boldsymbol{x}, \bar{x} ; \tau)$ serves as initial condition for real time propagation according to

$$
\begin{equation*}
G(\boldsymbol{x}, 0-i \tau ; \overline{\boldsymbol{x}}, 0-i \bar{\tau})=\mathrm{i}\left[G^{M}(\boldsymbol{x}, \bar{x} ; \tau)-G^{M}(\boldsymbol{x}, \bar{x} ;-\bar{\tau})\right] \tag{1.44}
\end{equation*}
$$

[^2]Instead of making the orbitals $\phi_{i}^{0}(\boldsymbol{x})$ time-dependent, it is advantageous to approach Eq. (1.41) using a static basis:

$$
\begin{equation*}
G(1, \overline{1})=\sum_{i, j=1}^{n_{b}} \phi_{i}^{0 *}(\boldsymbol{x}) \phi_{j}^{0}(\boldsymbol{x}) G_{i j}(t, \bar{t}) . \tag{1.45}
\end{equation*}
$$

Consequently, one is left with equations of motion for the elements $G_{i j}(t, \bar{t})=$ $-i\left\langle T_{\mathcal{C}} \hat{a}_{i}(t) \hat{a}_{j}^{\dagger}(\bar{t})\right\rangle$ which are just the Green's functions with respect to the creation (annihilation) operators $a_{i}^{\dagger}(t)\left(a_{i}(t)\right)$ of the steady state $i$ [31, 32]. In addition, the products of $H^{0}(\Sigma[G])$ and $G$ in Eq. (1.41) become standard matrix multiplications, and the time-dependent self-energy is evaluated in the manner of Eq. (1.37) as

$$
\begin{equation*}
\Sigma_{i j}[G](t, \bar{t})=-i \delta_{\mathcal{C}}(t-\bar{t}) \sum_{k, l=1}^{n_{b}}\left(w_{i j, k l}-w_{i l, k j}\right) G_{k l}^{<}(t, \bar{t}) \tag{1.46}
\end{equation*}
$$

We note that, using the Hartree-Fock approximation (1.46), it is fully sufficient to propagate the KBE for the center of mass (c.m.) time $t_{c . m .}=(t+\bar{t}) / 2$ alone, instead of expanding $G$ into the whole two-time plane $[0, t] \times[0, \bar{t}]$. However, this is no longer the case when higher-order self-energies $\Sigma[G]$ are involved-examples are second Born or $G W$ type formulas $[24,33]$ which are non-local in time and lead to correlation and memory effects [34].

Example. Let us consider two fermions of mass $m$ and charge $q$ confined in a one-dimensional (1D) parabolic trap $V\left(\boldsymbol{r}_{i}\right)=\frac{m}{2} \omega^{2} \boldsymbol{r}_{i}^{2}$ with frequency $\omega$ and $\boldsymbol{r}_{i} \rightarrow$ $\left(x_{i}, 0,0\right), i=1,2$. Due to the electrostatic charge both fermions repel each other via the Coulomb potential $w\left(x_{1}-x_{2}\right)=q^{2} /\left(4 \pi \epsilon_{0}\left|x_{1}-x_{2}\right|\right)$. However, in 1D it is convenient to apply a regularized Coulomb potential [35] with $\left|x_{1}-x_{2}\right|$ replaced by $\sqrt{\left(x_{1}-x_{2}\right)^{2}+\kappa^{2}}$. The parameter $\kappa>0$ keeps the integrals in Eqs. (1.33), (1.38) and (1.42) finite and, in a physical interpretation, allows for a transversal spread of the total wave function.

Using dimensionless units $\left\{x_{i} \rightarrow x_{i} / x_{0}, E \rightarrow E / E_{0}\right\}$ with $x_{0}=\sqrt{\hbar /(m \omega)}$ and $E_{0}=\hbar \omega$, the Hamiltonian reads

$$
\begin{equation*}
\hat{H}=\frac{1}{2}\left(-\nabla_{x_{1}}^{2}+x_{1}^{2}\right)+\frac{1}{2}\left(-\nabla_{x_{2}}^{2}+\bar{x}_{2}^{2}\right)+\frac{\lambda}{\sqrt{\left(x_{1}-x_{2}\right)^{2}+\kappa^{2}}} . \tag{1.47}
\end{equation*}
$$

Here, $\lambda=E_{C} / E_{0}=x_{0} / a_{B}$ is the coupling parameter-the ratio between the characteristic Coulomb energy $E_{C}=q^{2} /\left(4 \pi \epsilon_{0} x_{0}\right)$ [oscillator length $x_{0}$ ] and the confinement energy $E_{0}$ [Bohr radius $a_{B}=\left(4 \pi \epsilon_{0} \hbar \omega\right) / q^{2}$ ]. For fixed $\kappa$, the coupling parameter solely controls the system behavior. For $\lambda \ll 1$ (corresponding to high density), the two fermions will be found in a Fermi gas- or liquid-like state whereas in the (low-density) limit $\lambda \rightarrow \infty$, with $x_{0} \gg a_{B}$, quantum effects vanish in favor of classical, interaction dominated behavior. For moderate coupling $\lambda \gtrsim 1$, states with well localized density can be formed $[18,36]$. However, such structure formation strongly depends on the spin configuration.

In the following we examine the ground state and nonequilibrium situations of the two-fermion system (1.47) using the TDHF ansatz (1.30). Thereby, we further assume the orbitals $\phi_{1}$ and $\phi_{2}$ to be equal for all times $t$, i.e. we consider

$$
\begin{equation*}
\Psi\left(x_{1}, x_{2}, t\right)=\phi\left(x_{1}, t\right) \phi\left(x_{2}, t\right) \tag{1.48}
\end{equation*}
$$

This symmetric product (or singlet state) is justified as long as the spin wave function $\chi\left(\sigma_{1}, \sigma_{2}\right)$ is anti-symmetric.

With expression (1.48), the TDHF equations (1.32) simplify to a single equation for the orbital $\phi(x, t)$. In particular, it is easily seen that the exchange term in Eq. (1.33) becomes half the Hartree-potential, thus

$$
\begin{equation*}
\hat{\Sigma}(x, t)=\frac{1}{2} \int \mathrm{~d} \bar{x} 2|\phi(\bar{x}, t)|^{2} w(x-\bar{x}) \tag{1.49}
\end{equation*}
$$

In analogy to Eq. (1.37) for the ground state problem, the self-energy has to be modified to $\Sigma_{i j}[c]=\sum_{k l}\left(2 w_{i j, k l}-w_{i l, k j}\right) \varrho_{k l}[c]$ with the constraint $N \rightarrow N / 2$. A similar expression holds for the time-dependent case, Eq. (1.46). The initial state of the system is now obtained either by direct imaginary time propagation or by solving the Roothaan-Hall equations (1.35) for $\phi(x)=\phi_{1}^{0}(x)$, e.g. expanded in terms of oscillator eigenfunctions ${ }^{3} \varphi_{n+1}(x)=\left[2^{n} n!\sqrt{\pi}\right]^{-1 / 2} \mathrm{e}^{-x^{2} / 2} H_{n}(x)$ with $n=0,1,2, \ldots$. For the specific case of $\lambda=2$ and $\kappa=0.1$, Fig. 1.3 shows the result of both methods.

The imaginary time propagation starts from the energetically lowest oscillator eigenfunction $\varphi_{1}(x)$, which is the ideal reference state for $\lambda \equiv 0$; see the thin black curve for $t=0$ in Fig. 1.3 (a). Then, as time increases, $|\phi(x,-\mathrm{i} t)|^{2}$ evolves getting more and more broadened due to the Coulomb-like interaction (see the gray curves in Fig. 1.3 (a)) and, finally, it converges to a stationary solution $\phi_{t \rightarrow \infty}(x)$, denoted by the thick black curve. At the same time, the effective one-particle potential $V^{\text {eff }}$, defined as

$$
\begin{equation*}
V^{\mathrm{eff}}(x,-\mathrm{i} t)=V(x)+\Sigma[\phi](x,-\mathrm{i} t) \tag{1.50}
\end{equation*}
$$

changes from a sharply peaked function in space into a smoother stationary equilibrium potential $V_{t \rightarrow \infty}^{\text {eff }}(x)$; see the sequence of dashed curves. Fig. 1.3 (b) shows the (rapid) convergence of the different energies obtained from the total wave function $\Psi\left(x_{1}, x_{2}, t\right)$. Particularly, note that $E_{\text {pot }}$ is computed from the single-particle potential $V(x)$, whereas $E_{\mathrm{TDHF}}$ denotes the expectation value of $\Sigma[\phi](x,-\mathrm{i} t)$. According to the initial state $\varphi_{1}(x)$, the kinetic and potential energy at $t=0$ take the value of two independent particles in the 1D harmonic confinement, $E_{\text {kin }}=E_{\text {pot }}=\frac{1}{2}$, while the interaction energy $E_{\mathrm{TDHF}}$ is initially much larger than the converged value. For comparison, Fig. 1.3 also shows how the self-consistent field method. It reaches the same ground state in the limit $n_{b} \gtrsim 10$, cf. the orbitals $\phi_{1, n_{b}}^{0}(x)$ with $n_{b}=4,6,10$.

As an application to nonequilibrium, we consider the response of the two-fermion system to a short turn-off of the trap potential $V(x)$, where the switch-off time has been chosen to be $\delta t \approx 0.1$ and, hence, $V(x, t)=\theta(t-\delta t) V(x)$. After releasing the

[^3]

Fig. 1.5 Computation of the ground state function $\phi(x)(\lambda=2, \kappa=0.1)$ via imaginary time propagation starting from the lowest oscillator eigenstate $\varphi_{1}(x)$. (a) Orbital $\phi(x,-\mathrm{i} t)$ for different times $t$ and the corresponding effective one-particle potential $V^{\text {eff }}(x,-\mathrm{i} t)$; discretization $\Delta t=$ 0.01 and $\Delta x=0.04$. The thick black (dashed) line shows the converged result for $t \rightarrow \infty$. (b) Convergence of the different energy contributions. The thin dotted lines denote the (not yet converged) energies obtained from the self-consistent field method with $n_{b}=6$, compare with $\phi_{1, n_{b}}^{0}(x)$.
confinement, the initial product state of the two fermions is no longer an eigenstate of the actual system. Consequently, $\phi(x, t)$ undergoes damping and starts to oscillate harmonically when the confinement is reactivated for $t \geq \delta t$. In conjunction with this, the potential energy $E_{\mathrm{pot}}(t)$ as computed from the total wave function, also begins to oscillate with a frequency $\omega_{\mathrm{br}}$ which we call the breathing frequency. It is found that this frequency depends strongly on $\lambda$ as well as on the regularization parameter $\kappa$, cf. Fig. 1.3 (a) and (b). For $\lambda \rightarrow 0$, the breathing frequency approaches the value $\omega_{\mathrm{br}}=2 \omega$ which is the well-known result for the noninteracting (ideal) system [37]. With increasing $\lambda$, the frequency $\omega_{\text {br }}$ generally decreases in the considered $\lambda$-regime, and further exhibits a non-trivial behavior at moderate coupling, $\lambda \gtrsim 1$. A more detailed analysis of the breathing motion of quantum particles in traps can be found in [38].

### 1.4 Quantum Monte Carlo methods

The phenomenon of physical structure formation is closely related to the exact treatment of many-body correlations. To rigorously take into account the mutual interplay between a large number of individual particles, random-number-based


Fig. 1.6 Nonequilibrium response of the two-fermion system, Hamiltonian (1.47), after a short turn-off of the confinement. (a) Initial ground state $\left|\phi_{\lambda, \kappa}(x)\right|^{2}$ as a function on the coupling parameter $\lambda$ and $\kappa$. For the assignment of the four different curves with $\kappa=0.01,0.1,1.0$ and 10.0 see Fig. (b). For $\lambda \ll 1$, the ground state is practically independent of $\kappa$. (b) $\lambda$-dependence of the potential energy oscillation (breathing) frequency $\omega_{\mathrm{br}}$ for different $\kappa$ values in units of the confinement frequency $\omega$. The breathing frequency is obtained from a fit, $a \cos \left(\omega_{\mathrm{br}} t+b\right)+c$, applied to the time-dependent potential energy.

Metropolis Monte Carlo methods (MC) can be applied to efficiently sample the high-dimensional configuration space. Unlike molecular dynamics (see chapter by Ott et al. ), the Monte Carlo method is stochastic rather than dynamical and thus, following the general concept, only statistical averages of equilibrium properties can be computed. In this section we start the introduction with the basic Monte Carlo algorithm, which can also be used in advanced quantum simulations, as shown in the second part of this section. Here, the imaginary time path integral representation is derived, which allows for a (quasi-classical) high-temperature approximation of the $N$ particle density matrix and its numerical solution with efficient Monte Carlo methods.

### 1.4.1 Metropolis Monte Carlo Method

The original idea of this stochastic simulation method was coined by E. Fermi, J. von Neumann, S. Ulam, and N. Metropolis, who proposed in 1953 a stochastic algorithm to generate microstates according to the Boltzmann distribution, so that thermal averages could be computed easily [39]. This famous Metropolis sampling scheme has been rated as being among the top ten algorithms having the "greatest influence on the development and practice of science and engineering in the 20th century" [40].

To describe the considered model system, Eq. (1.1), by means of MC methods, the dynamical physical process has to be transformed into a stochastic one. A key element in the Metropolis Monte Carlo procedure is thus the concept of the Markov chain. This means that the immediate sequencing of a state depends only on the present state, regardless of the preceding development of the system. The Markov process generates a path in the configuration space and all quantities of interest are averaged along this trajectory, which is the probabilistic analogue to that generated by the equations of motion in molecular dynamics [42, 43] (see figure in chapter of Ott et al.).

In mathematical terms the Markov chain is defined as a sequence of sample points $i$ in the configuration space $\Omega$

$$
\begin{equation*}
\boldsymbol{r}_{0}^{N} \xrightarrow{W} \ldots \xrightarrow{W} \boldsymbol{r}_{i}^{N} \xrightarrow{W} \boldsymbol{r}_{i+1}^{N} \xrightarrow{W} \boldsymbol{r}_{i+2}^{N} \xrightarrow{W} \ldots, \tag{1.51}
\end{equation*}
$$

where the vector $\boldsymbol{r}_{i}^{N}=\left(\boldsymbol{r}_{1}, \boldsymbol{r}_{2}, \ldots, \boldsymbol{r}_{N}\right)_{i} \in \Omega$ of dimension $3 N$ comprises the coordinates of all $N$ particles. The transition operator $W\left(\boldsymbol{r}_{i}^{N} \rightarrow \boldsymbol{r}_{j}^{N}\right)$ has to obey the detailed balance condition [44]

$$
\begin{equation*}
P\left(\boldsymbol{r}_{i}^{N}\right) W\left(\boldsymbol{r}_{i}^{N} \rightarrow \boldsymbol{r}_{j}^{N}\right)=P\left(\boldsymbol{r}_{j}^{N}\right) W\left(\boldsymbol{r}_{j}^{N} \rightarrow \boldsymbol{r}_{i}^{N}\right), \tag{1.52}
\end{equation*}
$$

for each MC step from one to any other state. In thermal equilibrium at a fixed external heat bath temperature $T$, the probability $P\left(\boldsymbol{r}_{i}^{N}\right)$ of obtaining configuration $\boldsymbol{r}_{i}^{N}$ is weighted according to the Boltzmann probability distribution

$$
\begin{equation*}
P\left(\boldsymbol{r}_{i}^{N}\right)=\frac{1}{Z} \mathrm{e}^{-\beta E\left(\boldsymbol{r}_{i}^{N}\right)}, \tag{1.53}
\end{equation*}
$$

where $\beta=E_{0} / k_{\mathrm{B}} T$ is the dimensionless inverse temperature ${ }^{4}$, $k_{\mathrm{B}}$ is Boltzmann's constant, $E$ the (dimensionless) total system energy according to Hamiltonian (1.1) and $Z=\sum_{\Omega} \mathrm{e}^{-\beta E\left(\boldsymbol{r}_{i}^{N}\right)}$ the partition function of the canonical ensemble. Hence, the relative transition probability for the step $\boldsymbol{r}_{i}^{N} \rightarrow \boldsymbol{r}_{j}^{N}$ is a function of the total energy change $\Delta E=E\left(\boldsymbol{r}_{j}^{N}\right)-E\left(\boldsymbol{r}_{i}^{N}\right)$ only

[^4]\[

$$
\begin{equation*}
\frac{W\left(\boldsymbol{r}_{i}^{N} \rightarrow \boldsymbol{r}_{j}^{N}\right)}{W\left(\boldsymbol{r}_{j}^{N} \rightarrow \boldsymbol{r}_{i}^{N}\right)}=\mathrm{e}^{-\beta \Delta E} \tag{1.54}
\end{equation*}
$$

\]

This equation is satisfied by the Metropolis function [39]

$$
W\left(\boldsymbol{r}_{i}^{N} \rightarrow \boldsymbol{r}_{j}^{N}\right)= \begin{cases}\exp (-\beta \Delta E) & \Delta E>0  \tag{1.55}\\ 1 & \Delta E \leq 0\end{cases}
$$

This means that if a trial move $\boldsymbol{r}_{i}^{N} \rightarrow \boldsymbol{r}_{j}^{N}$ lowers the energy, then the step is always accepted. However, if the energy is increased, the trial step is accomplished with a probability $W<1$ only, and is otherwise rejected.

Starting from an arbitrary configuration $\boldsymbol{r}_{0}^{N} \in \Omega$, after an initial thermalization time of the simulation, the expectation value of the ensemble average of a generic physical quantity $A\left(\boldsymbol{r}^{N}\right)$ can be estimated as an arithmetic mean over the Markov chain of $K$ consecutive MC steps

$$
\begin{equation*}
\langle A\rangle=\sum_{i \in \Omega} P\left(\boldsymbol{r}_{i}^{N}\right) A\left(\boldsymbol{r}_{i}^{N}\right) \approx \frac{1}{K} \sum_{k=1}^{K} A\left(\boldsymbol{r}_{k}^{N}\right) . \tag{1.56}
\end{equation*}
$$

A central point in this context is the ergodicity of the Markov process, which refers to the condition that any state in the configuration space has to be accessible from any other state in a finite number of MC steps. An inherent problem with respect to the ergodicity in strongly correlated systems is, naturally, the (exponentially) growing autocorrelation time with the system size, which may easily exceed the simulation time. Especially at low temperatures one has to take care that the statistics are not biased, since the expectation values of the observed quantities may seem to have converged although the system is trapped in local minima and has barely moved in the configuration space $\Omega$. However, one should be aware that long simulation times do not automatically guarantee more accurate results generally, as discussed in reference [41].

Recommendable reviews on the subject of classical Monte Carlo simulations are to be found, for example, in Refs. [42, 43, 45, 46].

### 1.4.2 Path Integral Monte Carlo

The path integral Monte Carlo simulation (PIMC) technique is founded on R.P. Feynman's path integral formulation of quantum mechanics which, unlike E. Schrödinger's and W. Heisenberg's differential equation formalism, generalizes the formulation of classical mechanics, in particular Hamilton's principle of least action. In spite of its intuitive and theoretical sophistication, the evaluation of the path integrals is not at all trivial since one has to integrate over all possible states of the system for each moment in time [47].

In analogy to classical statistical mechanics, in which thermal equilibrium expectation values are defined as a canonical average of all microstates weighted by the Boltzmann factor (see Eq. (1.56)), the equilibrium state of a quantum system at a given inverse temperature, $\beta$, is fully characterized by the many-body density operator,

$$
\begin{equation*}
\hat{\rho}(\beta)=\frac{1}{Z} \mathrm{e}^{-\beta \hat{H}}=\frac{1}{Z} \sum_{n}\left|\psi_{n}\right\rangle \mathrm{e}^{-\beta E_{n}}\left\langle\psi_{n}\right| \tag{1.57}
\end{equation*}
$$

This statistical operator, $\hat{\rho}$, is defined as the superposition of pure $N$-particle eigenfunctions, $\left|\psi_{n}\right\rangle$, which are exponentially weighted with the allowed energy eigenvalues, $E_{n}$, determined from the stationary Schrödinger equation $\hat{H}\left|\psi_{n}\right\rangle=E_{n}\left|\psi_{n}\right\rangle$. This means that the density operator $\hat{\rho}$ mixes the pure states, $\left|\psi_{n}\right|^{2}$, according to the thermal distribution and thus generalizes the concept of the wave function to finite temperatures, i.e., mixed ensembles.

As seen in the chapter by Bonitz et al., the thermal average of an observable $\hat{A}$ in thermodynamic equilibrium is defined as

$$
\begin{equation*}
|\hat{A}|=\operatorname{Tr}[\hat{\rho} \hat{A}]=\sum_{i}\langle i| \hat{\rho} \hat{A}|i\rangle=\sum_{i, j}\langle i| \hat{\rho}|j\rangle\langle j| \hat{A}|i\rangle . \tag{1.58}
\end{equation*}
$$

If $\hat{A}$ is diagonal in the chosen basis, the thermal average can be determined from the diagonal elements of the density matrix only, i.e.,

$$
\begin{equation*}
\langle\hat{A}\rangle=\sum_{i}\langle i| \hat{\rho}|i\rangle A_{i} \tag{1.59}
\end{equation*}
$$

However, a direct computation of $\hat{\rho}$ requires knowledge of the complete energy spectrum by solving the $N$-particle Schrödinger equation, which, in most cases, is impossible for interacting systems. As we will see, we can avoid this problem by using a (path) integral representation of the $N$-particle density matrix, which can be evaluated efficiently with the help of numerical Monte Carlo methods.

To do so, we change into the basis of position vectors $\boldsymbol{r}^{N}=\left(\boldsymbol{r}_{1}, \boldsymbol{r}_{2}, \ldots, \boldsymbol{r}_{N}\right)$, in which the off-diagonal density matrix becomes a function of 6 N particle coordinates, i.e.,

$$
\begin{equation*}
\hat{\rho} \rightarrow \rho\left(\boldsymbol{r}^{N}, \boldsymbol{r}^{N^{\prime}} ; \beta\right) \equiv\left\langle\boldsymbol{r}^{N}\right| \mathrm{e}^{-\beta \hat{H}}\left|\boldsymbol{r}^{N^{\prime}}\right\rangle \tag{1.60}
\end{equation*}
$$

Note that in this position basis all particles are labeled. Moreover, the function values of the density matrix are positive ${ }^{5}$ for all of its arguments and have the significance of a probability for the transition from an initial state $\boldsymbol{r}^{N}$ to the final state $\boldsymbol{r}^{N^{\prime}}$. The non-negativity of the density matrix elements is an essential prerequisite for the subsequent application of Monte Carlo methods. In coordinate representation the (normalized) thermal average of operator $\hat{A}$ becomes

[^5]\[

$$
\begin{equation*}
\langle\hat{A}\rangle=\frac{1}{Z} \int \mathrm{~d} \boldsymbol{r}^{N}\left\langle\boldsymbol{r}^{N}\right| \rho \hat{A}\left|\boldsymbol{r}^{N}\right\rangle=\frac{1}{Z} \iint \mathrm{~d} \boldsymbol{r}^{N} \mathrm{~d} \boldsymbol{r}^{\prime N} \rho\left(\boldsymbol{r}^{N}, \boldsymbol{r}^{\prime N} ; \beta\right)\left\langle\boldsymbol{r}^{N}\right| \hat{A}\left|\boldsymbol{r}^{\prime N}\right\rangle, \tag{1.61}
\end{equation*}
$$

\]

and the partition function is written as

$$
\begin{equation*}
Z(\beta)=\int \mathrm{d} \boldsymbol{r}^{N} \rho\left(\boldsymbol{r}^{N}, \boldsymbol{r}^{N} ; \beta\right) . \tag{1.62}
\end{equation*}
$$

In general, these functional integrals cannot be carried out since an explicit analytical form of $\rho\left(\boldsymbol{r}^{N}, \boldsymbol{r}^{N^{\prime}} ; \beta\right)$ is commonly unknown for non-ideal quantum systems. To overcome this problem, we reduce the density matrix to the one known for free particles in the high-temperature limit. To this end we employ the product property of the density matrix

$$
\begin{equation*}
\hat{\rho}(\beta)=\mathrm{e}^{-\beta \hat{H}}=\underbrace{\mathrm{e}^{-\tau \hat{H}} \ldots \mathrm{e}^{-\tau \hat{H}}}_{M \text { times }}=\prod_{s=1}^{M} \hat{\rho}(\tau), \quad M \tau=\beta, \tag{1.63}
\end{equation*}
$$

which allows us to expand a low-temperature density matrix into a series of density matrices at $M$ times higher temperature, $\tau$. Insertion of $M-1$ high-temperature factors gives us the density matrix in position basis as

$$
\begin{align*}
\rho\left(\boldsymbol{r}^{N}, \boldsymbol{r}^{N^{\prime}} ; \beta\right) & =\left\langle\boldsymbol{r}^{N}\right| \mathrm{e}^{-\beta \hat{H}}\left|\boldsymbol{r}^{N^{\prime}}\right\rangle \\
& =\left\langle\boldsymbol{r}^{N}\right| \prod_{s=1}^{M} \mathrm{e}^{-\tau \hat{H}}\left|\boldsymbol{r}^{N^{\prime}}\right\rangle \\
& =\int \cdots \int \mathrm{d} \boldsymbol{r}_{1}^{N} \mathrm{~d} \boldsymbol{r}_{2}^{N} \ldots \mathrm{~d} \boldsymbol{r}_{M-1}^{N} \prod_{s=0}^{M-1}\left\langle\boldsymbol{r}_{s}^{N}\right| \mathrm{e}^{-\tau \hat{H}}\left|\boldsymbol{r}_{s+1}^{N}\right\rangle \\
& =\int \cdots \int \mathrm{d} \boldsymbol{r}_{1}^{N} \mathrm{~d} \boldsymbol{r}_{2}^{N} \ldots \mathrm{~d} \boldsymbol{r}_{M-1}^{N} \prod_{s=0}^{M-1} \rho\left(\boldsymbol{r}_{s}^{N}, \boldsymbol{r}_{s+1}^{N} ; \tau\right), \tag{1.64}
\end{align*}
$$

where the ordered set $\left(\boldsymbol{r}_{0}^{N}, \boldsymbol{r}_{1}^{N}, \ldots, \boldsymbol{r}_{M}^{N}\right)$ represents a path in configuration space. Expression (1.64) is exact and comprises in the limit $M \rightarrow \infty$ an integration over all possible paths through configuration space linking the fixed initial and final points, $\boldsymbol{r}_{0}^{N}=\boldsymbol{r}^{N}$ and $\boldsymbol{r}_{M}^{N}=\boldsymbol{r}^{N^{\prime}}$.

Interestingly, in the position basis many observables $\hat{A}$ are diagonal, which implies that only diagonal elements of the full (low-temperature) density matrix, $\rho(\beta)$, are relevant, see Eq. (1.59). As a result, the partition function, Eq. (1.62), now becomes an integral that runs over closed paths

$$
\begin{equation*}
Z(\beta)=\int \cdots \int \mathrm{d} \boldsymbol{r}_{1}^{N} \mathrm{~d} \boldsymbol{r}_{2}^{N} \ldots \mathrm{~d} \boldsymbol{r}_{M-1}^{N} \prod_{s=0}^{M-1} \rho\left(\boldsymbol{r}_{s}^{N}, \boldsymbol{r}_{s+1}^{N} ; \tau\right), \quad \boldsymbol{r}_{0}^{N}=\boldsymbol{r}_{M}^{N}, \tag{1.65}
\end{equation*}
$$

and is determined by the off-diagonal elements of the high-temperature density matrices $\rho(\tau)$.

Considering the system in question, cf. Eq. (1.1), the Hamiltonian consists in its general form,

$$
\begin{equation*}
\hat{H}=\hat{K}+\hat{V} \tag{1.66}
\end{equation*}
$$

of two non-commuting $N$-particle operators, the kinetic $\hat{K}$ and the potential $\hat{V}$ operators with $[\hat{K}, \hat{V}] \neq 0$. Expansion yields a cumbersome expression for the exponential operator

$$
\begin{align*}
\mathrm{e}^{-\tau(\hat{K}+\hat{V})} & =\mathrm{e}^{-\tau \hat{K}} \mathrm{e}^{-\tau \hat{V}} \mathrm{e}^{-\frac{\tau^{2}}{2}[\hat{K}, \hat{V}]} \mathrm{e}^{-\frac{\tau^{3}}{6}[[\hat{V}, \hat{K}], \hat{K}+2 \hat{V}]}+\mathcal{O}\left(\tau^{4}\right)  \tag{1.67a}\\
& =\mathrm{e}^{-\tau \hat{K}} \mathrm{e}^{-\tau \hat{V}} \mathrm{e}^{-\frac{\tau^{2}}{2}[\hat{K}, \hat{V}]}+\mathcal{O}\left(\tau^{3}\right)  \tag{1.67b}\\
& =\mathrm{e}^{-\tau \hat{K}} \mathrm{e}^{-\tau \hat{V}}+\mathcal{O}\left(\tau^{2}\right) \tag{1.67c}
\end{align*}
$$

However, Trotter's product formula states that for self-adjoint operators $\hat{K}$ and $\hat{V}$ (which are bounded from below in a Hilbert space) in the limit of a large number of high-temperature factors, $M \rightarrow \infty$, the total density matrix (1.63) can be approximated as a simple product of potential and kinetic density matrices by neglecting the commutators from the exact operator identity (1.67), i.e.,

$$
\begin{align*}
\hat{\rho}(\beta) & =\mathrm{e}^{-\beta(\hat{K}+\hat{V})}=\left[\mathrm{e}^{-\tau(\hat{K}+\hat{V})}\right]^{M} \stackrel{!}{=} \lim _{M \rightarrow \infty}\left[\mathrm{e}^{-\tau \hat{K}} \mathrm{e}^{-\tau \hat{V}}\right]^{M}  \tag{1.68}\\
& =\left[\mathrm{e}^{-\tau \hat{K}} \mathrm{e}^{-\tau \hat{V}}\right]^{M}+\mathcal{O}\left(M^{-1}\right)
\end{align*}
$$

Note that the validity of the approximation made for finite $M$ in the last step of Eq. (1.68) is not at all obvious due to the propagation of the error terms with respect to $\tau=\beta / M[48,49]$. The error of the high-temperature representation is therefore strongly affected by the number of high-temperature factors, $M$. Hence, the issue of convergence involving finite $M$ has to be checked carefully for each particular system under study.

The high-temperature matrix element $\rho\left(\boldsymbol{r}_{s}^{N}, \boldsymbol{r}_{s+1}^{N} ; \tau\right)$ in Eqs. (1.64) and (1.65) can be approximated as

$$
\begin{align*}
\rho\left(\boldsymbol{r}_{s}^{N}, \boldsymbol{r}_{s+1}^{N} ; \tau\right) & \equiv\left\langle\boldsymbol{r}_{s}^{N}\right| \mathrm{e}^{-\tau(\hat{K}+\hat{V})}\left|\boldsymbol{r}_{s+1}^{N}\right\rangle \approx\left\langle\boldsymbol{r}_{s}^{N}\right| \mathrm{e}^{-\tau \hat{K}} \mathrm{e}^{-\tau \hat{V}}\left|\boldsymbol{r}_{s+1}^{N}\right\rangle  \tag{1.69}\\
& =\mathrm{e}^{-\tau V\left(\boldsymbol{r}_{s}^{N}\right)}\left\langle\boldsymbol{r}_{s}^{N}\right| \mathrm{e}^{-\tau \hat{K}}\left|\boldsymbol{r}_{s+1}^{N}\right\rangle
\end{align*}
$$

where $\hat{V}$ is diagonal in the spatial coordinate representation. The kinetic energy density matrix elements of free particles are obtained by a momentum eigenstate expansion

$$
\begin{align*}
\left\langle\boldsymbol{r}_{s}^{N}\right| \mathrm{e}^{-\tau \hat{K}}\left|\boldsymbol{r}_{s+1}^{N}\right\rangle & =\int \mathrm{d} \boldsymbol{p}^{N}\left\langle\boldsymbol{r}_{s}^{N} \mid \boldsymbol{p}^{N}\right\rangle \exp \left[-\tau \sum_{i=1}^{N} \frac{\hat{\boldsymbol{p}}_{i}^{2}}{2 m_{i}}\right]\left\langle\boldsymbol{p}^{N} \mid \boldsymbol{r}_{s+1}^{N}\right\rangle  \tag{1.70}\\
& =\lambda_{M}^{-3 N} \exp \left[-\frac{\pi}{\lambda_{M}^{2}}\left(\boldsymbol{r}_{s}^{N}-\boldsymbol{r}_{s+1}^{N}\right)^{2}\right]
\end{align*}
$$

Here we take advantage of the diagonality of the kinetic operator $\hat{K}=\sum_{i=1}^{N} \frac{\hat{\boldsymbol{p}}_{i}{ }^{2}}{2 m_{i}}$ in momentum space, and note that the Gaussian type integral can be evaluated analytically after explicit expressions for the plane waves $\left\langle\boldsymbol{r}_{s}^{N} \mid \boldsymbol{p}^{N}\right\rangle$ and $\left\langle\boldsymbol{p}^{N} \mid \boldsymbol{r}_{s+1}^{N}\right\rangle$ have been substituted. The term $\lambda_{M}=\sqrt{2 \pi \hbar^{2} \beta / m M}$ denotes the thermal DeBroglie wave length. Insertion of the high-temperature matrices (1.69) and (1.70) into Eq. (1.64) provides us the discrete time path integral representation of the $N$-particle density matrix

$$
\begin{align*}
& \rho\left(\boldsymbol{r}^{N}, \boldsymbol{r}^{N^{\prime}} ; \beta\right) \approx \int \cdots \int \mathrm{d} \boldsymbol{r}_{1}^{N} \mathrm{~d} \boldsymbol{r}_{2}^{N} \ldots \mathrm{~d} \boldsymbol{r}_{M-1}^{N} \\
& \quad \times \lambda_{M}^{-3 N} \exp \left(-\frac{\pi}{\lambda_{M}^{2}} \sum_{s=0}^{M-1}\left(\boldsymbol{r}_{s}^{N}-\boldsymbol{r}_{s+1}^{N}\right)^{2}\right) \exp \left(-\tau \sum_{s=0}^{M-1} V\left(\boldsymbol{r}_{s}^{N}\right)\right) \tag{1.71}
\end{align*}
$$

which is valid for quantum systems with the Hamiltonian (1.66) and a quadratic dispersion law for $\boldsymbol{k}=\boldsymbol{p} / \hbar$.

Following the analogy between Feynman's original idea of a time-evolution operator $\hat{U}\left(t, t^{\prime}\right)=\mathrm{e}^{-\mathrm{i} \hat{H} t / \hbar}$ and the definition in Eq. (1.57), the inverse temperature $\beta$ may be considered as imaginary time, where $t \rightarrow \beta \hbar / i$ and the imaginary time step is $\tau=\beta / M$. Thus, the set of coordinates $\boldsymbol{r}_{s}^{N}$ at a specific integer number $s=1 \ldots M-1$ are commonly named "imaginary time slice", since only particle images within the same slice, $\boldsymbol{r}_{s}^{N}$, interact with each other via the weakened (iso-time) potential $v\left(\boldsymbol{r}_{s}^{N}\right)=V\left(\boldsymbol{r}_{s}^{N}\right) / M$, see figure 1.7. The classical-like particle images in successive slices $\left\{\boldsymbol{r}_{s}^{N}, \boldsymbol{r}_{s+1}^{N}\right\}$ are linked by a spring-like energy term, which is due to the quadratic quantum mechanical kinetic energy of the free particle and ensures a finite particle extension. Hence, in the imaginary-time path integral formulation a quantum system becomes mapped onto a classical one such that each physical (quantum) particle is represented by a path through $M$ positions (here called particle images) in configuration space at different values in imaginary time. This path forms a classical ring polymer of $M$ links. Depending on the inverse temperature $\beta$ and particle mass $m$, the spring coupling becomes more or less rigid and, consequently, the quantum particles become more or less delocalized.

Most of the thermodynamic quantities are determined by the trace of the density matrix (1.71), i.e., closed imaginary time trajectories from $\boldsymbol{r}^{N}$ to $\boldsymbol{r}^{N^{\prime}}=\boldsymbol{r}^{N}$. For instance the probability $p\left(\boldsymbol{r}^{*}\right)$ to observe an arbitrary particle at position $\boldsymbol{r}^{*}$ is given as arithmetic average over the imaginary time paths of all $N$ particles as

$$
\begin{equation*}
p\left(\boldsymbol{r}^{*}\right)=\frac{1}{N M} \sum_{i=1}^{N} \sum_{s=0}^{M-1}\left\langle\delta\left(\boldsymbol{r}^{*}-\boldsymbol{r}_{s}^{i}\right)\right\rangle_{\rho_{N}} \tag{1.72}
\end{equation*}
$$



Fig. 1.7 Sketch on Feynman's path integral representation of a trapped 2D quantum system with three electrons. The probability density $p(x, y)$ is obtained by mapping of the beads along the imaginary time paths onto the 2D plane.
where $\langle\ldots\rangle_{\rho_{N}}$ defines the thermodynamic average according to Eq. (1.61).
So far, only quantum systems composed of distinguishable spinless particles (boltzmannons) have been considered. However, even in the case in which the Hamiltonian does not explicitly depend on particle spin, inclusion of quantum statistics requires sampling of the particle permutations in addition to the integrations in coordinate space. Specifically, the many-body density matrix (1.71) has to be properly symmetrized with respect to an arbitrary exchange of two indistinguishable bosons (e.g. bosonic atoms, molecules or excitons), i.e.,

$$
\begin{equation*}
\rho^{S}\left(\boldsymbol{r}^{N}, \boldsymbol{r}^{N^{\prime}} ; \beta\right)=\frac{1}{N!} \sum_{P}(+1)^{P} \rho\left(\boldsymbol{r}^{N}, \hat{P} \boldsymbol{r}^{N^{\prime}} ; \beta\right) \tag{1.73}
\end{equation*}
$$

or antisymmetrized under arbitrary exchange of two indistinguishable fermions (such as electrons or holes with the same spin projection), i.e.,

$$
\begin{equation*}
\rho^{A}\left(\boldsymbol{r}^{N}, \boldsymbol{r}^{N^{\prime}} ; \beta\right)=\frac{1}{N!} \sum_{P}(-1)^{P} \rho\left(\boldsymbol{r}^{N}, \hat{P} \boldsymbol{r}^{N^{\prime}} ; \beta\right) \tag{1.74}
\end{equation*}
$$

where $\hat{P}$ is the permutation operator for particle indices and $P$ is the parity of the permutation. In the framework of path integral theory, the permutations can be
decomposed into a sequence of two-particle exchanges along the imaginary timepath. The pair exchanges are carried out by the transposition of particle positions in particular time slices, from which the paths of several particles can be merged into a single one. Such multi-particle trajectories correspond to off-diagonal elements of the density matrix, but still form closed loops.

The superposition of all $N$ ! permutations of $N$ identical particles leads to the inherent (numerical) fermion sign problem since the alternating sign of the prefactor in the case of fermions, Eq. (1.74), causes an essential cancellation of positive and negative contributions corresponding to even and odd permutations, respectively. Thus, an accurate calculation of such vanishing differences is strongly complicated by the increase of quantum degeneracy arising at low temperatures and high densities, where all permutations appear with equal probability.

The high-dimensional convolution integrals of the density matrix, Eqs. (1.71), (1.73), and (1.74), over $3 N(M-1)$ degrees of freedom ${ }^{6}$ can be numerically evaluated by a slightly modified version of the Metropolis sampling algorithm outlined for the classical systems. However, to reduce computational effort and increase the efficiency of Monte Carlo sampling, various sophisticated move strategies (e.g. the multi-level bisection sampling method or the worm algorithm [50]), approximations for the pair density matrix (e.g. using matrix-squaring technique [51, 52]), fast converging estimators with less statistical variance and many further improvements have been developed over the last decades. For further (technical) details on this subject, we refer the interested reader to the following recommended in-depth references [44, 45, 53, 54, 55].

### 1.5 Summary

In this tutorial we have provided an introduction to time-dependent and timeindependent quantum simulations. The former part split up into an exact treatment of the one-particle time-dependent Schrödinger equation, and also an approximate investigation of many-body systems on the basis of Hartree-Fock theory (and beyond). With these two techniques, all quantum effects, e.g. tunneling, quantization, interference phenomena, can be well described and simulated to any desired accuracy. Furthermore, no approximations to external fields, such e.g. laser fields, trapping potentials, have to be introduced. The TDSE is exact for both, particles of fermionic and bosonic character, whereas the Hartree-Fock method and its improvements as described here, is well suited for fermionic calculations and is often used in quantum chemistry. The (exact) many-body wave function is here reduced to an (approximate) one-particle function which contains all pertinent information about the system under investigation. The extraction of physical properties is often a challenging task and much attention has to be paid to this point. On the other hand, the wave function based time-dependent Schrödinger equation methods are limited to one particle in

[^6]a single-active electron approach, where the possible effects of additional particles are only included by utilizing effective external fields. Of course, such methods offer high accuracy in regard to one particle, but lack other many-body effects.

In the last part of this tutorial, we presented an introduction to the field of quantum Monte Carlo techniques. This method allows for the accurate calculation of equilibrium state properties of many-body systems with no further approximations, i.e. inclusion of all correlation effects. The main advantage lies in the (efficient) sampling of the density matrix, which especially allows for a large number of bosonic particles. However, no phase information or corresponding wave function can be constructed in this way. Hence, this method is not suitable for investigating excitations and dynamics. fermionic calculations are, up to now, limited to small systems due to the fermionic sign problem.

## References

1. W. Press, W. Vetterling, S. Teukolsky, B. Flannery, Numerical Recipes (Cambridge University Press, 2002)
2. W. van Dijk, F. M. Toyama: preprint arXiv:physics/0701150v1 (2007)
3. K. Boucke, H. Schmitz, H.-J. Kull: Phys. Rev. A 56763 (1997)
4. D. Bauer, P. Koval: Comp. Phys. Comm. 174, 396-421 (2005)
5. D. Neuhauser, M. Baer: J. Chem. Phys. 90 4351-4355 (1989)
6. A. Vibok, G. G. Balint-Kurti: J. Chem. Phys. 96 8712-8719 (1992)
7. Xue-Shen Liu, Xiao-Yan Liu, Zhong-Yuan Zhou, Pei-Zhu Ding, Shou-Fu Pan, Int. J. Quant. Chem., 79 343-349 (2000)
8. H.-J. Kull, V. T. Tikhonchuk: Phys. Plas. 12063301 (2005)
9. S. Bauch: Diploma thesis, University of Kiel (2008), http://www.theo-physik.uni-kiel.de/ bonitz/theses.html
10. G.D. Mahan, Many-Particle Physics, 2nd ed. (Plenum Press, New York, 1990)
11. P.A.M. Dirac, Proc. Cam. Phil. Soc. 26, 376 (1930)
12. K.R. Sandhya Devi, and S.E. Koonin, Phys. Rev. Lett. 47, 27 (1981)
13. M.A. Ball, A.D. McLachlan, Molecular Physics 7, 501 (1963)
14. K.C. Kulander, Phys. Rev. A 36, 2726 (1987)
15. N.E. Dahlen, and R. van Leeuwen, Phys. Rev. A 64, 023405 (2001)
16. M. Bonitz, Quantum Kinetic Theory (B.G. Teubner, Stuttgart, 1998)
17. W.D. Kraeft, D. Kremp, W. Ebeling, and G. Röpke, Quantum Statistics of Charged Particle Systems (Akademie Verlag, Berlin, 1986)
18. K. Balzer, and M. Bonitz, J. Phys. A: Math. Theor. 42, (2009)
19. M. Bonitz, D. Kremp, D.C. Scott, R. Binder, W.D. Kraeft, and H.S. Köhler, J. Phys.: Condens. Matter 8, 6057 (1996)
20. H. Ehrenreich, and M.H. Cohen, Phys. Rev. 115, 786 (1959)
21. N.H. Kwong, M. Bonitz, R. Binder and S. Köhler, phys. stat. sol. (b) 206, 197 (1998)
22. J. Caillat, J. Zanghellini, M. Kitzler, O. Koch, W. Kreuzer, and A. Scrinzi, Phys. Rev. A 71, 012712 (2005)
23. M.A.L. Marques, and E.K.U. Gross, Annu. Rev. Phys. Chem. 55, 427 (2004)
24. L.P. Kadanoff, and G. Baym, Quantum Statistical Mechanics (Benjamin, Inc., New York, 1962)
25. P. Echenique, J.L. Alonso, Mol. Phys. 105, 3057-3098 (2007)
26. P. Ludwig, K. Balzer, A. Filinov, H. Stolz, and M. Bonitz, New. J. Phys 10, 083031 (2008)
27. C.C.J. Roothaan, Rev. Mod. Phys. 20, 69 (1951); G.G. Hall, Proc. R. Soc. (London) A205, 451 (1951)
28. L.V. Keldysh, Zh. Eksp. Teor. Fiz. 47, 1515 (1964) [Sov. Phys. JETP 20, 235 (1965)]
29. N.E. Dahlen, and R. van Leeuwen, J. Chem. Phys. 122, 164102 (2005)
30. K. Balzer, M. Bonitz, R. van Leeuwen, N.E. Dahlen, and A. Stan, submitted to Phys. Rev. B; arXiv:cond-mat/08102425 (2008)
31. N.E. Dahlen, and R. van Leeuwen, Phys. Rev. Lett. 98, 153004 (2007)
32. K. Balzer, Diploma thesis, Kiel University (2007) http://www.theo-physik.uni-kiel.de/~bonitz/theses.html
33. A. Stan, N.E. Dahlen, and R. van Leeuwen, Europhys. Lett. 76, 298 (2006)
34. R. Binder, H.S. Köhler, and M. Bonitz, Phys. Rev. B 55, 5110 (1997)
35. K. Jauregui, W. Häusler, and B. Kramer, Europhys. Lett. 24, 581-587 (1993)
36. A.V. Filinov, M. Bonitz, and Yu.E. Lozovik, Phys. Rev. Lett. 86, 3851 (2001)
37. M. R. Geller, and G. Vignale, Phys. Rev. B 53, 6979 (1996); G. Watanabe, Phys. Rev. A 73, 013616 (2006)
38. S. Bauch, K. Balzer, D. Hochstuhl, and M. Bonitz, to be published (2009)
39. N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller, and E. Teller, Equation of state calculation by fast computing machines, Journal of Chemical Physics 21, 1087 (1953)
40. J. Dongarra and F. Sullivan, Guest Editors Introduction to the top 10 algorithms, Computing in Science \& Engineering 2, 22 (2000)
41. J. Böning, A. Filinov, P. Ludwig, H. Baumgartner, M. Bonitz, and Yu.E. Lozovik, Melting of trapped few particle systems, Phys. Rev. Lett. 100, 113401 (2008)
42. D.W. Heermann, Computer Simulation Methods in Theoretical Physics, 2nd edition SpringerVerlag New York, Berlin, Heidelberg (1990)
43. K. Binder, Computersimulationen, Physik Journal 5, 25 (2004)
44. A. Filinov, J. Böning, and M. Bonitz, Path Integral Monte Carlo Simulations of Charged Particles in Traps, Chapter in: Springer Lecture Notes in Physics 739, 397 (2008)
45. M. Bonitz and D. Semkat (eds.), Introduction to Computational Methods for Many-Body Physics, Rinton Press, Princeton (2006)
46. W. Janke, Monte Carlo Methods in Classical Statistical Physics, Chapter in: Springer Lecture Notes in Physics 739, 79 (2008)
47. R.P. Feynman and A.R. Hibbs, Quantum Physics and Path Integrals, McGraw-Hill, New York (1965)
48. H.F. Trotter, Approximation of semi-groups of operators, Pacific J. Math. 8, 887 (1958)
49. H. De Raedt and B. De Raedt, Applications of the generalized Trotter formula, Physical Review A 28, 3575 (1983)
50. M. Boninsegni, N. Prokof'ev, and B. Svistunov, Worm Algorithm for Continuous-Space Path Integral Monte Carlo Simulations, Phys. Rev. Lett. 96, 070601 (2006)
51. R.G. Storer, Path-Integral Calculation of the Quantum-Statistical Density Matrix for Attractive Coulomb Forces, J. Math. Phys. 9, 964 (1968)
52. A.D. Klemm and R.G. Storer, The structure of quantum fluids: helium and neon, Australian Journal of Physics 26, 43 (1973)
53. D.M. Ceperley, Path integrals in the theory of condensed helium, Reviews of Modern Physics 67, 279 (1995)
54. B. Militzer, Path Integral Monte Carlo Simulations of Hot Dense Hydrogen, Ph.D. thesis, University of Illinois at Urbana-Champaign (2000)
55. L.B. i Barberà, Path Integral Monte Carlo. Algorithms and applications to quantum fluids, Ph.D. thesis, Universitat Politècnica de Catalunya (2002)
56. D.M. Ceperley, Fermion Nodes, J. Stat. Phys. 63, 1237 (1991)
57. V.S. Filinov, M. Bonitz, W. Ebeling, and V.E. Fortov, Thermodynamics of hot dense H-plasmas: Path integral Monte Carlo simulations and analytical approximations, Plasma Physics and Controlled Fusion 43, 743 (2001)
58. V. Filinov, H. Fehske, M. Bonitz, V.E. Fortov, and P.R. Levashov, Correlation effects in partially ionized mass asymmetric electron-hole plasmas, Phys. Rev. E 75, 036401 (2007)
59. C.H. Mak, R. Egger, and H. Weber-Gottschick, Multilevel Blocking Approach to the Fermion Sign Problem in Path-Integral Monte Carlo Simulations, Phys. Rev. Lett. 81, 4533 (1998)
60. M.V. Dikovsky and C.H. Mak, Analysis of the multilevel blocking approach to the fermion sign problem: Accuracy, errors, and practice, Phys. Rev. B 63, 235105 (2001)
61. B. Jakob, P.-G. Reinhard, C. Toepffer, and G. Zwicknagel, Wave packet simulation of dense hydrogen, Phys. Rev. E 76, 036406 (2007)
62. Robert E. Wyatt, Quantum Dynamics with Trajectories, Series: Interdisciplinary Applied Mathematics (2005)
63. V. Filinov, M. Bonitz, A. Filinov, and V. Golubnychiy, Wigner Function Quantum Molecular Dynamics, Chapter in: Springer Lecture Notes in Physics 739, 41 (2008)
64. P.N. Roy, S. Jang, and G.A. Voth, Feynman path centroid dynamics for Fermi-Dirac statistics, J. Chem. Phys. 111, 5303 (1999)
65. W.D. Kraeft, D. Kremp, W. Ebeling, and G. Röpke, Quantum Statistics of Charged Particle Systems, Akademie-Verlag, Berlin (1986)
66. M. Bonitz, Quantum Kinetic Theory, Teubner-Verlag, Stuttgart/Leipzig (1998)
67. M. Bonitz, D. Semkat, A. Filinov, V. Golubnychiy, D. Kremp, D.O. Gericke, M.S. Murillo, V. Filinov, V.E. Fortov, W. Hoyer, and S.W. Koch, Theory and Simulation of Strong Correlations in Quantum Coulomb Systems, J. Phys. A: Math. Gen. 36, 5921 (2003)

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[^1]:    ${ }^{1}$ For simplicity, we suppress the Planck quantum $\hbar$ in Eqs. (1.28) and (1.29) as well as in the remainder of this chapter.

[^2]:    ${ }^{2}$ The field operators satisfy the equal-time anti-commutation relations $\left[\hat{\psi}_{H}(\boldsymbol{x}, t), \hat{\psi}_{H}^{\dagger}(\overline{\boldsymbol{x}}, t)\right]_{+}=$ $\delta(\boldsymbol{x}-\overline{\boldsymbol{x}})$ and $\left[\hat{\psi}_{H}^{(\dagger)}(\boldsymbol{x}, t), \hat{\psi}_{H}^{(\dagger)}(\overline{\boldsymbol{x}}, t)\right]_{+}=0$, where $[\hat{A}, \hat{B}]_{+}=\hat{A} \hat{B}+\hat{B} \hat{A}$.

[^3]:    ${ }^{3} H_{n}(x)$ denotes the Hermite polynomial of order $n$.

[^4]:    ${ }^{4} E_{0}$ and $l_{0}$ are base units of energy and length, e.g., in trapped systems the harmonic oscillator ground state energy $E_{0}=\hbar \omega_{0}$ and oscillator length $l_{0}=\sqrt{\hbar /\left(m \omega_{0}\right)}$. A dimensionless system of units is obtained by applying the transformation rules $\left\{r \rightarrow r / r_{0}, E \rightarrow E / E_{0}\right\}$.

[^5]:    ${ }^{5}$ Here, we do not yet consider the problematic issue of Fermi statistics.

[^6]:    ${ }^{6}$ We typically use numbers of high-temperature factors $M$ in the range $100 \leq M \leq 300$.

