Quantum Mechanics Simulated as Branching Process

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Diffusion processes with branching play an important role in statistical dynamics. They are a common approach to the computing of quantum mechanical groundstates, 1,2 and serve as models for population dynamics and as physical pictures for biological evolution, 3,4.

On a computer the efficiency of this simulation method is limited by the approach to the infinitesimal time step, which is necessary to perform alternating diffusion and branching steps.

In this paper, a method is described, which eliminates the infinitesimal time step for a certain class of branching processes, if the process of interest can be “embedded” into another process, which is solvable by other analytic and/or numerical methods. The simplest choice for the embedding process is given by a process with a constant branching rate, which dominates the rate of the embedded process.

I. INTRODUCTION

A population of random–walkers \( \phi(x,t) \) which independently move, multiply and die shall be described by an equation of motion where the movement is given by a diffusion process, while the branching process depends on the spatial coordinate \( x \). The probability for either a birth or a death process occurring during an infinitesimal time–intervall \([t,t+dt]\) in the spatial interval \([x,x+dx]\) is given by \( |S(x)|\phi(x,t)\,dt\,d^d x \,dt \), where \( S(x) < 0 \) denotes decay processes and \( S(x) > 0 \) denotes birth processes.

\[
\text{Pr}\{ a \text{ birth process occurs during } [t,t+dt] \} = \begin{cases} 
0, & \text{if } S(x) < 0, \\
S(x)\phi(x,t)\,dt\,d^d x, & \text{if } S(x) > 0,
\end{cases}
\]

\[
\text{Pr}\{ a \text{ decay process occurs during } [t,t+dt] \} = \begin{cases} 
-S(x)\phi(x,t)\,dt\,d^d x, & \text{if } S(x) < 0, \\
0, & \text{if } S(x) > 0.
\end{cases}
\]

To stress the close relation to imaginary time quantum–mechanics the reproduction operator \( S \) is introduced as the negative potential \( S(x) = -V(x) \). The simplest case, where the the diffusion is homogeneous and isotropic the dynamics is governed by the equation

\[
\partial_t \phi(x,t) = \{ \partial_x^2 - V(x) \} \phi(x,t)
\]

This equation is equivalent to an imaginary time SCHRÖDINGER–equation, with the dynamics

\[
- \hbar \partial_t \phi = -H \phi.
\]

The formal analogy between imaginary time SCHRÖDINGER–equation and statistical physics has been studied since 3,5, a contemporary approach is given in 6. Most of the works focuses on the relation between the imaginary time SCHRÖDINGER–equation and equilibrium statistics. However, this paper emphasises, that there is a more natural interpretation as a non–equilibrium process, which has been explicitly stated in 7 and which is implicitly used in 8.

II. THEORETICAL FOUNDATION FOR THE IMAGINARY TIME SCHRÖDINGER–EQUATION

In this section, the method to measure the energy of the quantum–mechanical groundstate and to stabilize the population shall be derived. In contrast to the common bilinear product \( \langle \phi|H|\phi \rangle \), a flux through the population shall be used to measure the energy. The population is stabilized on the average, by subtracting the groundstate energy \( E_0 \), which is determined “on the run”.

A. Formal solution

In analogy to real time SCHRÖDINGER–equation \( -i\hbar \phi = H \phi \) can be solved using the same eigen–function system \( \psi_n \) of \( H \) with \( H\psi_n = E_n \psi_n \). This way one obtains exponentially growing (decaying) contributions for \( E_i < 0 \) \( (E_i > 0) \), instead of oscillating ones

\[
\phi(x,t) = \sum_n c_n e^{-E_i t} \psi_n(x), \quad c_n = \langle \phi_0 | \psi_n \rangle.
\]
Of course, the groundstate $\psi_n$ grows faster (or decays slower) than all other states and will dominate the ensemble for $t \to \infty$, thus on the long run the normalised population converges to the quantum–mechanical groundstate
\[
\psi_0(x) = \lim_{t \to \infty} \phi(x,t) = \int \phi(x',t) dx'.
\] (8)

B. Measuring the energy

It is remarkable, that the energy of $\phi$ is related to a flux through the population, which is defined on an area $G$ by
\[
F(t) = \int_G H\,d\phi = -\int_{\partial G} \nabla \phi \, dn + \int_G \phi \, d^2x.
\] (9)

Obviously, an exploding or decaying system cannot be in equilibrium. Of course, even if the total population is stable $\int_G \phi(x,t) = \text{constant}$, there are areas, where the random–walkers are born, and other areas reached by diffusion, where they die. Thus, the RDS cannot be related to an equilibrium system. However, under certain conditions it is convenient to have a stationary flux, which is equivalent to a system with a stable population.

C. Stabilizing the population

The main idea to stabilize the population is to determine the energy of the groundstate and to subtract it from the effective dynamics. This has the effect of putting the lowest eigen–value to zero by hand. As $\phi$ is the formal solution of
\[
\phi(t) = \exp (-Ht) \phi(0),
\] (10)
it is useful to notice, that for an arbitrary time–depending function $\bar{E}(t)$ the equation
\[
\partial_t \phi(x,t) = \{ \bar{E}(t) - H \} \phi(x,t),
\] (11)
with the same $c_n$ as defined in equation (3), is solved by
\[
\phi(x,t) = \sum_n c_n e^{\int_0^t \bar{E}(t') \, dt' - E_n t} \psi_n(x).
\] (12)
Thus, $\phi$ can also be stabilised by subtracting an average energy with the property $\int_0^t \bar{E}(t') \, dt' \approx E_0 t$, for $t \to \infty$, which is automatically implied if $\lim_{t \to \infty} \bar{E}(t) = E_0$. Therefore, the average
\[
\bar{E}(t) = \int_0^t F(t') \, dt' / \int_0^t \int_G \phi(x',t') \, dx' \, dt',
\] (13)
is chosen converging $\bar{E}(t) \to E_0$ because $\phi \to \psi_0$ for $t \to \infty$ by (8) and inserting $\phi$ into definition (3).

III. SIMULATION WITHOUT INFINITESIMAL TIME–STEPS

The starting point is the common time–step algorithm. The simulation needs $N$ time–steps to evolve from time $t = 0$ to the final time $T$, each step of length $\varepsilon = T/N$. With Rnd and $\xi$ denoting standard uniform and normal random–numbers the simplest formulation is:

For $n \leftarrow 0$ to $N$
1. $t \leftarrow n\varepsilon$,
2. move $x_r \leftarrow x_r + \sqrt{\varepsilon} \xi$,
3. if $|S(x_r)|\varepsilon > \text{Rnd}$ then perform a birth ($S > 0$) or death ($S < 0$) process,
4. next $n$.

At first, it is assumed, that there is an upper bound $\bar{S} > S(x)$ allowing to split step 3 into two parts:
3a. if $|\bar{S}|\varepsilon < \text{Rnd}$ reject any branching, next $n$,
3b. if $|S(x_r)| < \text{Rnd} \bar{S}$ then perform a birth ($S > 0$) or death ($S < 0$) process.

The probability of a branching event is the probability $p_a = |\bar{S}|\varepsilon$ to pass step 3a times the probability $p_b = |S(x_r)|\bar{S}$ to pass step 3b without rejection. The result is the correct branching rate $p_ap_b = |S(x_r)|\varepsilon$.

Now there is an inner loop, 1–3a, and an outer loop, 1–3b. In the inner loop there is no need to evaluate the exact branching potential $S(x)$. The probability, not to leave the inner loop after one step is $Q^1 = (1 - \bar{S}\varepsilon)$. The probability, not to leave the inner loop after $n$ steps, or equivalent until time $t = n\varepsilon$ is given by $Q^n = (1 - \bar{S}\varepsilon)^n = q_e(t)$. The limit $\varepsilon \to 0$ can be evaluated
\[
q_e(t) = (1 - \bar{S}\varepsilon)^{t/n} \xrightarrow{\varepsilon \to 0} \left( e^{-\bar{S}} \right)^t = e^{-\bar{S}t}.
\] (14)

Thus the whole loop can be replaced by:
while $t < T$
1. draw an exponentially distributed random–number $\tau \leftarrow \log (1 - \text{Rnd}) / \bar{S}$, $t \leftarrow t + \tau$
2. move $x_r \leftarrow x_r + \sqrt{\tau} \xi$,
3. if $|S(x_r)| < \text{Rnd} \bar{S}$ then perform a birth ($S > 0$) or death ($S < 0$) process,
4. next exponential time step.

This way, the time $\tau$ between to proposed branchings is related to the upper bound $\bar{S}$ for the potential $|S(x)|$, if the branching has been succeeded or rejected. The rate for evaluating the true $S(x)$ is $\bar{S}$, which can be chosen to be of a typical order of magnitude for the given problem. According to the considerations to stabilise the groundstate, section (II C), we choose $S(x,t) = \bar{E}(t) - V(x)$.

Although, the proof of the algorithm has not been given for time dependent $S(x,t)$, this generalisation is obvious. Furthermore, in the long time limit, the fluctuations of $\bar{E}(t)$ fade away.
IV. THE REPRESENTATION OF THE WAVE FUNCTION

The simulations have been performed by ensembles of $R$ independent random–walkers, each described by two variables, the coordinate $\xi_n$ and the time $\theta_n$, where and when the $r$–th walker has been a “candidate” for its $n$–th branching process, independent of a branching has been performed or not. Since the last branching proposal at time at location the random–walker has done a free random–walk. When it is considered asing proposal at time at location the random–walker has been performed or not. Since the last branch-
ing has been performed or not. Since the last branch-

\[ \phi(x, t) = \sum_{r=1}^R g(x - \xi_r, t - \theta_r) \]  

and averaging the flux $[\mathcal{F}]$ reduces to the computation and summation of integrals

\[ \int_0^t F(t') dt' = \sum_{r=1}^R \sum_{\nu \in \mathcal{D}} U(\theta_n - \theta^\nu_n, \xi^\nu_n) \]

with $U(\tau, \xi) = \int dt' \int d^d \varphi V(\varphi) g(\varphi - \xi, t')$.  

V. EXAMPLES

The quality of the simulations depends on the computation of $U(\tau, x)$. For all standard potentials like polynomials and COULOMB–like potentials, including interacting electronic systems, $U$ can be solved analytically.

A. Polynomials and the harmonic oscillator

In $[\mathcal{U}]$ the function $U(\tau, x)$ has been defined as the time average of the energy. For an arbitrary polynomial $P(x) = \sum_{k_1, \ldots, k_d} q_{k_1, \ldots, k_d} \prod_{i=1}^d x_i^{k_i}$ one finds

\[ U(t, x) = \sum_{k_1, \ldots, k_d} q_{k_1, \ldots, k_d} \prod_{i=1}^d \kappa_{j_i, k_i} t^{j_i+1} x_i^{k_i-j_i} \]  

with $\kappa_{j, k} = \frac{1+(-1)^{k}}{2} \left( \frac{k}{j} \right) \left( \frac{-1}{j/2} \right) \left( \frac{j}{j/2+1} \right)$ which is easy to implement. For the $d$–dimensional harmonic oscillator $V(x) = P(x) = \frac{1}{2} |x|^2$, one obtains the simple result

\[ U(t, x) = \frac{1}{2} t |x_0|^2 + \frac{d}{4} t^2. \]  

FIG. 1. paths of the harmonic oscillator for a single random–walker, $x' \pm \sqrt{t - \theta_n}$ to demonstrate the variance of the normal distribution. The diffusion is free for a time $\tau$ of the order of a typical time scale.

B. The COULOMB–potential

Although the COULOMB $1/|x|$ singularity has no upper bound, the function $U$ can also be computed by analytical methods.

By scaling the HAMILTONIAN gets $H = -\frac{i}{2} \partial_x^2 + \alpha/|x|$ with the SOMMERFELD–constant $\alpha$ being the only free parameter, thus $E_0 = -\frac{i}{2} \alpha^2$. The integrals $[\mathcal{U}]$ are solved in polar coordinates performing the integrations in the order $\varphi \rightarrow \theta \rightarrow r \rightarrow t$, with the angles defined according to the axis $0 \rightarrow x$. The $U_H$–function reads

\[ U_H(t, x) = \alpha \sqrt{2t} u \left( \frac{|x|}{\sqrt{2t}} \right), \]  

with $u(x') = (1/(2x') + x') \text{erf}(x') + e^{-x'^2} / \pi - x'$. The function $u(x')$ has a very simple structure, and is tabulated at the beginning of each run. The integrals evaluated for the computation of the COULOMB–potential may easily be generalised to simulate the ortho–helium atom. The HAMILTONIAN

\[ H = -\sum_{i=1}^2 \left( \frac{i}{2} \partial_{x_i}^2 - 2\alpha/|x_i| \right) + \alpha |x_1 - x_2| \]  

allows a separation of the $6 + 1$–dimensional integration. For $V_i = 2\alpha/|x_i|$ there is one integration for $x_i$ and another one for the coordinate which $V_i$ is independent of. The $V_{12} = \alpha/|x_1 - x_2|$ integration may be transformed into the centre of mass system, resulting in a constant factor and another integration for the relative coordinates which reduces to a COULOMB–integration again. The final result reads

\[ U_{He}(t, (x_1, x_2)) = 2 \sum_{i=1}^2 U_H(t, x_i) + U_H(t, x_1 - x_2). \]
VI. THE QUALITY OF THE RESULTS

To keep the number of random–walkers constant, every time a random–walker multiplies (dies) another one dies (multiplies) with probability $1/(R-1)$. For this “antagonist” the actualization of the coordinates has to be carried out, too. This way, $R$ does no fluctuate any more, otherwise the fluctuations of $R$ would cause a diffusion process of $R$, which is avoided for convenience.

![Graph](image)

**FIG. 2.** Systematic error of $E_0$ for the hydrogen atom, depending on the number of random–walkers. The straight line represents $1/R$.

The antagonist rule introduces an unknown additional coupling among two walkers considered as independent. This results in a $R^{-1}$ law, the large number of $R-1$ possible partners weakens the individual coupling. Thus the order of the systematic error is higher than the statistical error of $R^{-1/2}$ and can be neglected, if $R$ is sufficiently large (Fig. 3). Typical values are 0.1 percentage error for $R = 2^{10} = 1024$.

For harmonic or COULOMB potentials using a constant $\dot{S}(x,t)$ the condition $\dot{S} > S(x)$ is violated. However, due to the fast decay of the wave function this error decays exponentially fast for the harmonic oscillator. For the COULOMB like problems it only affects a negligible area. Fig. 3 gives an impression of two typical runs for the helium problem approaching the experimental groundstate energy better than 0.1%.

VII. CONCLUSION

The algorithm has proved its capability to simulate imaginary time SCHRODINGER–equations very efficient and accurate. The method of embedding has been extended to all problems, which can be formulated as branching processes, and it has been generalised to arbitrary time depending rates $S(x,t)$.

One interesting property of the algorithm for quantum–mechanics is the fact, that COULOMB 2–particle integrals can be solved analytically. Its importance is limited by the question, if it will be possible to extend it to fermionic systems. For all kinds of COULOMB–systems an identity like (21) holds as well and the singularities may be integrated and smoothed out. At least, it should be possible to introduce the nodes of a related problem as absorbing boundaries similar to (3).

However, the main advantage is opposite to (21) that there is no need of a “guiding wave function”. Therefore, the algorithm is easier to implement. The related ideas concerning fermionic systems and excited states could be applied as well.

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