

# Time evolution for quantum systems at finite temperature

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## Abstract

This paper investigates a new formalism to describe real time evolution of quantum systems at finite temperature. A time correlation function among subsystems will be derived which allows for a probabilistic interpretation. Our derivation is non-perturbative and fully quantized. Various numerical methods used to compute the needed path integrals in complex time were tested and their effectiveness was compared. For checking the formalism we used the harmonic oscillator where the numerical results could be compared with exact solutions. Interesting results were also obtained for a system that presents tunneling. A ring of coupled oscillators was treated in order to try to check selfconsistency in the thermodynamic limit. The short time distribution seems to propagate causally in the relativistic case. Our formalism can be extended easily to field theories where it remains to be seen if relevant models will be computable.

# 1 Introduction

Our aim in this work is to develop a non-perturbative formalism that combines real time and finite temperature for a full quantized theory. Actually, it makes little physical sense to talk about time evolution for *the whole system at a finite temperature* (as we would like to avoid using an abstract external heat bath). So it will be important to keep in mind that we want to study time-correlations among small subsystems of the full quantum system, of which we only know that the large system is in a *thermal state*. The formalism will show its consistency if these correlations tend to a fixed limit, in the thermodynamic limit of large full systems.

The original motivation was the understanding of real time processes at intermediate  $T$ 's due to instanton tunneling [1, 2], important within some field theories to obtain baryogenesis or quark deconfinement. The scope has been enlarged as we realize that one can pose similar questions in many areas of Physics or Chemistry, where one would like to get time correlations of some degrees of freedom for quantum systems at a given temperature. For example, the tunneling rate in ammonia molecules at finite  $T$ , or spin  $t$ -correlations in Ising-like solids.

We will assume that the quantum system is in a *thermal state* described by a density matrix  $\rho$  at time zero. We make then a first measurement on one (or a few) degrees of freedom, the applied operator being a projector onto the subspace compatible with the first measurement. We assume here, as in usual quantum mechanics, that the “collapse of the wave function” in the measurement process, can be described well enough by the non-unitary projection operator. To effectively reduce the *kets* and *bras* of  $\rho$  to the measured subspace, the projector has to be applied on both sides. A time  $t$  later, we make another measurement of some observable through the corresponding projector. We will show that the correlation function defined in this way has a nice and proper transition probability interpretation. This probability is gotten by multiplying the probabilities to be in quantum states (according to  $\rho$ ) by the probability to go from these states (projected onto some states of the subsystem) to some states at a later time.

This contrasts with the usual way to estimate time correlations by just computing thermal expectations of operators at two times, as derived for example from the linear response theory [3]. We will show that those expressions differ from ours if  $\rho$  doesn't commute with the projector, and do not have a probability interpretation. In the classical limit the operators commute and both expressions are equivalent.

Usually, at finite  $T = 1/\beta$ , one just takes the trace over Euclidean time  $\beta$  to calculate expectation values, which is relatively simple to compute with Feynman Path Integrals. For time correlations we will need a circuit in the complex time plane of the shape:  $(0 + i0) \rightarrow (t - i\epsilon) \rightarrow (0 - 2i\epsilon) \rightarrow (0 - i\beta)$ . The measured time correlations will be obtained by inserting suitable operators at the points  $(0 + i0)$ ,  $(t - i\epsilon)$  and  $(0 - 2i\epsilon)$ . The Path Integrals needed for this complex  $t$  will still be doable and converge with various methods, as we will show in the paper. In Section 2 the formalism will be developed and a representation in terms of the Path Integral formalism in „complex” time will be given. Section 3 outlines and compares three

numerical methods to do this integration. Section 4 treats some solved models like the harmonic oscillator, a double well, or the interesting case of a ring of  $N$  coupled oscillators. Finally Section 5 summarizes the results and gives an outlook over projected advancements.

## 2 Real time formalism

The question we want to ask is: what is the probability for some observed degrees of freedom, of a large quantum system at finite temperature, to make a transition to some other observed values after a time  $t$ . We will show that this probability is given by a product of three Green's functions in the complex  $(t, \beta)$  plane, as indicated in Fig.1, where one integrates over all unobserved variables. The whole expression can be casted into a Feynman Path Integral with periodic paths on the complex time circuit.

To fix ideas, let us ask for the probability,  $P_t^\beta(x_1, y_1)$ , that if the first particle (of a system of  $N$  interacting quantum particles) is located close to  $x_1$  at  $t = 0$ , it will be close to  $y_1$  at time  $t$ , the system being at temperature  $T = 1/\beta$ .

In order to deduce  $P_t^\beta(x_1, y_1)$ , we start from the knowledge that for  $t = 0$  the system is in a *mixed state*, described by the thermal density matrix:

$$\rho = \exp(-\beta H) = \sum_n \exp(-\beta E_n) |n\rangle \langle n|, \quad (1)$$

with the additional condition that the first degree of freedom be around  $x_1$ , which is obtained by applying the projector

$$P_{x_1} := \int_{x_1-a}^{x_1+a} dx_1 |x_1\rangle \langle x_1| * I_{2,\dots,N} \quad (2)$$

on both sides of  $\rho$ . The  $I_{2,\dots,N}$  means the identity operator for the coordinates 2 to  $N$ . Note that we have to take a small window  $[x_1 - a, x_1 + a]$  around  $x_1$  as otherwise we would measure the position with infinite precision implying total delocalization afterwards (we can see this effect numerically, in that the  $P_t^\beta(x_1, y_1)$  goes to a constant in  $y_1$  for very small windows), with the projector still satisfying  $P_{x_1}^2 = P_{x_1}$ . So, for  $t = 0$  we describe the system by

$$P_{x_1} \rho P_{x_1}. \quad (3)$$

This operator evolves in time as usual,

$$U_t^+ (P_{x_1} \rho P_{x_1}) U_t \quad \text{with } U_t = \exp(-iHt). \quad (4)$$

We measure again at time  $t$ , with a position  $y_1$  for the first particle. The probability is then:

$$P_t^\beta(x_1, y_1) = \frac{1}{\text{Norm.}} \text{Tr} \left\{ P_{y_1} U_t^+ (P_{x_1} \rho P_{x_1}) U_t \right\} \quad (5)$$

where we have discarded one of the  $P_{y_1}$  due to the cyclicity of the trace. This equation has the right probabilistic interpretation as we will see. The normalization can be taken so that the integration over  $y_1$  in Eq.(3) is one, corresponding to the assumption that the particle *is* in the window  $[x_1 - a, x_1 + a]$ , or with  $Z$ , in which case we include the a priori probability to be in that window. In both cases the integrated  $P_t^\beta$  is  $t$ -independent.

Using energy eigenfunctions to perform the trace in Eq. (5), one obtains an expression which allows a simple probabilistic interpretation:

$$\begin{aligned} P_t^\beta(x_1, y_1) &= \int_{x_1-a}^{x_1+a} dx_1 dx'_1 \int_{i=2, \dots, N} dy_i dx_i dx'_i \sum_n \exp(-\beta E_n) \langle n | x_i \rangle \langle x_i | U_t | y_i \rangle \langle y_i | U_t^\dagger | x'_i \rangle \langle x'_i | n \rangle \\ &= \int_{i=2, \dots, N} dy_i \sum_n \exp(-\beta E_n) \left| \int_{x_1-a}^{x_1+a} dx_1 \int_{i=2, \dots, N} dx_i G_t(y_1, y_i; x_i, x_1) \psi_n(x_1, x_i) \right|^2 \end{aligned} \quad (6)$$

This means (as mentioned above) that the *probability* to be on an energy level becomes multiplied by the *probability* to move from this level at the  $\vec{x}$ 's, to the position states at  $\vec{y}$ . Note that all the amplitudes from within the window  $x_1$  and the other  $x_i$  can interfere with each other as allowed in Quantum Mechanics, as we have not measured them more precisely. In contrast, the final  $\vec{y}$ 's could all have been precisely measured, but we chose not to measure them in Statistical Mechanics, so they all add as probabilities.

It should be mentioned that the correlation function used frequently in linear response theory (see ref. [1]),

$$\langle Q(t)Q(0) \rangle_\beta := \text{Tr}\{\exp(-\beta H)Q(t)Q(0)\}, \quad (7)$$

cannot be interpreted in this way, i.e. as a transition probability. Notice that if these  $Q$ 's were projection operators Eq. 7 and Eq. 5 would coincide in the classical limit, where  $P_{x_1}$  and  $\rho$  commute. But in the quantum case if one neglects one of the projectors, there is a mixing of amplitudes from terms coming from different energy states in the thermal mixture, which is clearly incorrect. In fact Eq. 7 does not even give a real positive number. If one uses  $|Q(t) - Q(0)|^2$  instead, which is positive per construction, it still doesn't have a probability interpretation. It should be mentioned that even if one starts from Eq. 7, one needs similar complex t-plane circuits to Fig. 1, as shown by Semenoff, Niemi, Weiss, Kobes and others [4], when deducing the relevant Feynman perturbation rules.

The evaluation of Eq.(5) can also be done by using position eigenfunctions, in which case we obtain a product of three Green's functions ( $G_\beta G_t^\dagger G_t$ ):

$$P_t^\beta(x_1, y_1) = \int_{x_1-a}^{x_1+a} dx_1 dx'_1 \int_{i=2, \dots, N} dx_i dx'_i dy_i \langle x_1, x_i | \rho | x'_1, x'_i \rangle \langle x'_1, x'_i | U_t^\dagger | y_1, y_i \rangle \langle y_1, y_i | U_t | x_1, x_i \rangle \quad (8)$$

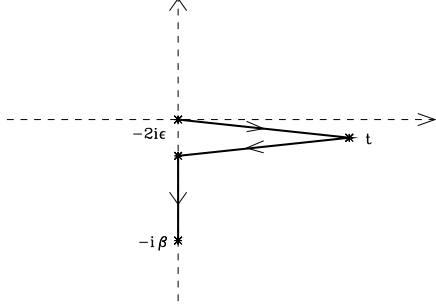


Figure 1: Propagation in complex time

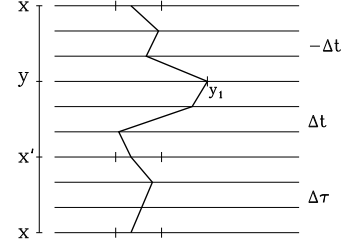


Figure 2: one possible path in complex time

This expression is in general easier to evaluate than Eq. 6, as it includes at once all of the energy eigenfunctions. This product of three Green's functions represents a propagation in "complex" time, as shown in fig. 1 (The  $\epsilon$  will be introduced in Sec. 3.2, here it is set to  $0_+$ ). Each Green function can be calculated by a Feynman Path Integral, but the product of the three can also be expressed by one Path Integral with constrained paths at the windows for the appropriate times as seen in fig. 2 (the paths are unconstrained in the other not shown dimensions).

The generalization to a field theory is in principle immediate, in fact it is being worked out for the 1+1 Quantum Ising model [9], where one is interested in the spatial and time correlations of spins at several temperatures.

### 3 Numerical Methods

When using Eq. 8, one has to evaluate the Green's functions and perform the integrations. It is well known that the Monte Carlo method can be used for the calculation of the temperature Green's function (i.e. for imaginary times). Numerical methods for the calculation of real time Greens functions are still rare. One method for their calculation, which one of us (E.M.) developed recently, and two other methods were implemented and tested. In the following we will present them and discuss their comparative (dis-)advantages.

We will start always from the real time path integral representation of the Greens functions:

$$G_t(y, x) = \int \mathcal{D}x \mathcal{D}p e^{i \int_0^t dt (p\dot{q} - H(p, q))} \quad (9)$$

For two of the methods we will integrate out the momenta to get the usual:

$$G_t(y, x) = \int \mathcal{D}x \, e^{iS[x(t)]} \quad (10)$$

To compute this expression we have to consider discrete  $\Delta t$  and check the convergence to infinitesimal  $dt$ . The analytical continuation to Euclidean times can be easily obtained by taking  $\Delta\tau = i\Delta t$  in eq. 9. Actually we can take  $\Delta\tau$  to be a fully complex number and move diagonally in the complex  $t$ -plane. In fact it will be useful for improving convergence to take slightly slanted lines  $(\Delta t - i\Delta\epsilon)$  for the real time propagation (where  $\epsilon/\Delta\epsilon = N_t$  steps) .

### 3.1 Matrix Method

This method was first proposed by Dullweber, Hilf and Mendel in [5]. They have shown that this method works for both real and imaginary times. The basic idea consists in considering the propagator for short times  $\Delta t$  only among discrete points in  $x$ -space, therefore replacing the path integration by matrix multiplications with itself. It was interesting to observe that the method converged, even for real times, with reasonably fine spatial discretizations ( $\Delta x < \Delta t/10$ ) . The short time propagator matrix reads:

$$K_{ij}(\Delta t) \approx \left( \frac{m}{2\pi i \Delta t} \right)^{1/2} e^{i \left[ \frac{m}{2} \left( \frac{x_{t+\Delta t}^i - x_t^j}{\Delta t} \right)^2 - V(\bar{x}) \right] \Delta t} \quad (11)$$

Here one only needs the short time Lagrangian instead of the action as a function of the end-points. The discretization in space delivers the indexation for the matrix  $K(\Delta t)$ . In this way we obtain

$$G_t = [K(\Delta t)]^N (\Delta x)^{N-1}. \quad (12)$$

Using  $n$  successive matrix quadratures we obtain larger times according to  $t = \Delta t * (2^n)$ . From our numerical experience this has been the fastest method. It is the best one to study systems at deep temperature or their long time behaviour. On the other hand these matrices do become very large if the system has too many degrees of freedom needing large amounts of memory.

### 3.2 Monte Carlo Method

The path integration could be replaced by a summation over randomly generated paths, with a Metropolis weighting for the Euclidean pieces of the action. (It is possible to choose right from the beginning paths for the product of the three Greens functions). But this summation will not converge, as the amplitudes for the real time Greens functions all have the same absolute value and differ only by their phases. This situation can be improved by introducing a small

imaginary part  $-i\epsilon$  into the time propagation, so that the paths get a weight and can be made to converge (to the right answer). One has to be careful though in taking the limit  $\epsilon \rightsquigarrow 0$  as in this process the Monte Carlo convergence gets rapidly worse. The effect of this  $\epsilon$  is easily seen to be

$$\exp \left\{ iS^{\Delta t - i\Delta\epsilon} \right\} = \exp \left\{ -\Delta\epsilon H \right\} \exp \left\{ iS^{\Delta t} \right\} \quad (13)$$

where we have neglected terms of  $O(\Delta\epsilon^2)$  and where the superscripts in the actions mean the time intervals over which we integrate. This means that paths with very high energy are exponentially suppressed. Unfortunately the convergence slows down rapidly in the  $\epsilon$  to 0 limit. It does not seem to be reasonable to use this method for more than 2 or 3 steps of  $dt$ , but low temperatures can be reached. Nevertheless it is the method of choice if one is limited in some problem by computer memory, as it needs the least with this method.

### 3.3 Fast Fourier Transform Method

Here one starts from the path integration over phase space in eq. 9, as explained in Ref. [6]. After discretization of space and time, the Greens function can be written as the succession of two Fourier Transforms per time step (we have generalized their folding with a given wave function):

$$G_{\Delta t}(x_1, \tilde{x}_0) = \int dp_1 dx_0 \exp \left\{ i \left( p_1(x_1 - x_0) - \frac{p_1^2 \Delta t}{2m} - V(x_1, x_0) \Delta t \right) \right\} \delta(x_0 - \tilde{x}_0) \quad (14)$$

$$= \mathcal{F}^{-1} \left[ \hat{T} \mathcal{F} \left[ \hat{V} \delta(x_0 - \tilde{x}_0) \right] \right] \quad (15)$$

Here  $\mathcal{F}$  means Fourier Transform and  $\hat{T}$  and  $\hat{V}$  are the exponentiated kinetic/potential energies, respectively. In other words, the propagator for one time step from a fixed position  $\tilde{x}_0$  to some arbitrary point  $x_1$  is achieved by a twofold Fourier transform, each of which can be computed effectively with the Fast Fourier Transform (FFT) method. Iterative application of this operator  $\mathcal{F}^{-1} \hat{T} \mathcal{F} \hat{V}$  yields the propagator for more time steps (only one  $\Delta t$  gain in one iteration in contrast to the matrix method).

For general potentials  $V(x_1, x_0)$ , where the "mid point rule" is hard to disentangle (for the FFT), it is better to use the alternative discretization:

$$\exp(V(x_1, x_0)) \rightsquigarrow \exp(V(x_1)/2) \exp(V(x_0)/2) \quad (16)$$

where the term in  $x_1$  can be extracted to the front of the fourier transforms above.

Here too an  $\epsilon$  can improve the results, as the fourier transform assumes the transformed function to be periodic and an imaginary  $\epsilon$  forces the exponentiated energies to fulfill this requirement.

This method has moderate RAM requirements as only vectors have to be stored, but the computational time increases linearly with the number of  $\Delta t$ 's. In principle this method should be faster than the matrix method in problems with higher number of degrees of freedom, but in practice this remains to be seen as the FFT has to be done for each of the "spectator" coordinate anew and the overhead for each FFT compared with a matrix multiplication is considerable.

## 4 Solved models

### 4.1 Harmonic Oscillator

We applied these methods to compute time evolution in quantum systems at finite temperature to a variety of systems. We will first treat the harmonic oscillator as the evolution of the probability distribution can be compared in this case with analytical results. Let us assume that a particle in a harmonic oscillator potential (with  $\omega = 1, m = 1$ ) is for  $t = 0$  in the interval  $[-1.25; -0.25]$  (this starting interval is indicated by a horizontal line in fig. 3). The evolution of the probability density is depicted at three times, so that one can imagine the wave packet oscillating in the potential. Note that the wave packet at  $t = 3.04 \approx \pi - 0.1$  is (as expected) symmetric to the distribution at  $t = 0.1$ . The extreme broadening at the intermediate time is due to the chosen high temperature, so that also energy eigenfunctions of higher levels contribute to the result. If we decrease the temperature, we obtain a more localized probability distribution. To make sure that our correlation function reproduces indeed the behaviour of a h.o. the movement of the mean of the probability distribution was calculated (fig. 4). The result is a cosine, with somewhat larger oscillation amplitude for a higher temperature, as expected.

For this model with just one degree of freedom, the coherence of the signal is maintained (with contributions from various states), as in these simple cases each mode does not get perturbed by others, the Boltzmann distribution of states being simply postulated. In more complex systems, for which this formalism is really being developed, the other degrees of freedom of the system form the heat bath for the degree of freedom which is being measured and this simple coherence will be lost. In the case of many degrees of freedom, the thermodynamic limit should be consistent with the Boltzmann distribution.

The Green's functions for the h.o. are explicitly known (see e.g. [7]), so one can assess the three numerical methods of Sec. 3. The Monte-Carlo method seems to be unsuitable for more than 2-3 time-steps, even with a fairly large  $\epsilon$ . Apart from that, it converges well for low temperatures (i.e. large numbers of  $d\tau$ ) with little RAM requirement. Better results and with smaller errors due to the  $\epsilon$  convergence factors are obtained with the other two methods. For large times the matrix method is the fastest, even though larger amounts of memory have to be used.

As a last test we proved that the total probability turns out to be conserved, to a good approximation for discrete  $\Delta x$ , as expected.



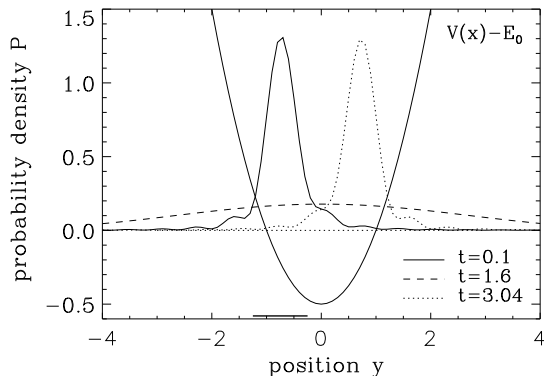


Figure 3: Probability to be at  $y$  for an h.o. for times  $t \approx 0, \pi/2$  and  $\pi$ , at  $T = 1$ . Exact Green's functions were used.

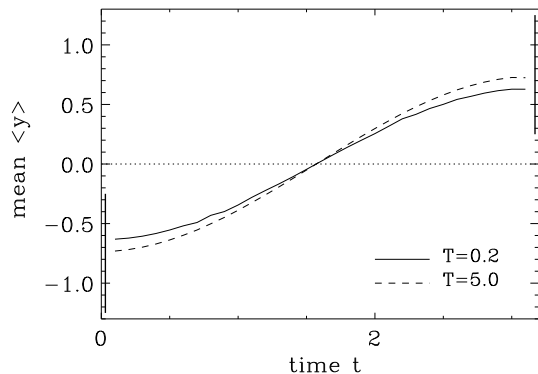


Figure 4: Mean of the wave-packet as a function of time, two temperatures. Vertical bars are the initial (mirrored) windows.

## 4.2 Double Well Potential

Here we wanted to study quantum tunneling at finite temperature. We used a nearly box shaped  $x^6$ -potential with an added Gaussian barrier (height  $E_{max} = 30$ ). Let us first look at the low  $T$  case. At  $t = 0$  the particle is in a window located on the left side. Fig. 5 shows the temporal evolution. The horizontal bar is again the initial interval. If only the lowest two energy levels contribute reasonably to the distribution, the result is a nearly 100 % tunneling after a time  $T_{\text{tun}} \approx \frac{\pi}{E_1 - E_0}$ , and due to the symmetry half of its periodicity. Fig. 6 shows the total probability to be on the right half as a function of time for several temperatures. The periodicity of the low- $T$ -case ( $T_{\text{tun}} \approx 10$ ) is apparent. If there are higher wavefunctions that interfere, this property is destroyed and the total probability after some time to be on each side tends to  $1/2$ .

While for higher  $T$  there is a sizable probability to be on an energy level above the potential barrier, this is not the case for low  $T$  (e.g.  $T \approx 0.156$ :  $p(E > 30) < 10^{-78}\%$ ). Thus, semiclassical perturbation theory as in [2], [8] cannot be used here. Their ansatz (*for calculating sphaleron-rates in electroweak field theory*) was to start with a quantum thermal ensemble of field configurations and then calculate the classical time evolution for each of them. Thus only sphaleron-like transitions to other minima are possible. But for temperatures far below the sphaleron-energy the behaviour of the system is governed by tunneling processes and therefore the calculation must be fully "quantum".

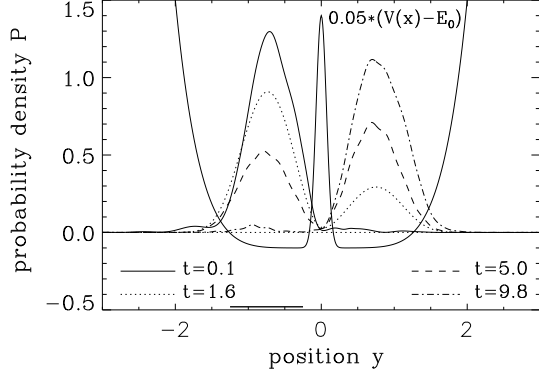


Figure 5: Probability to be at some  $y$  for a double well for a low temperature.

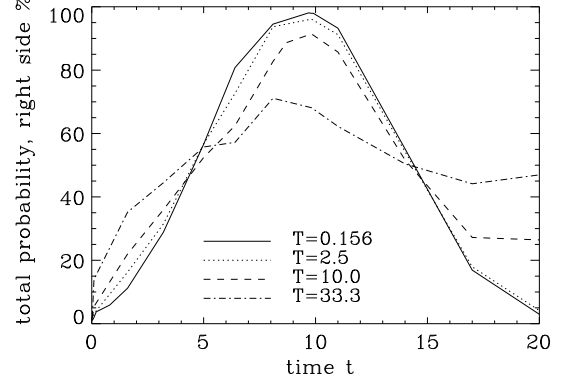


Figure 6: Total Probability to be in the right side well as a function of time for different temperatures.

### 4.3 N coupled oscillators

The most interesting case that we have solved in this work is the  $N$  particle chain of coupled oscillators on a circle, with transversal oscillations. This is the first genuine finite temperature system that we treated in the sense that the other degrees of freedom form a heat bath for the measured one. We have been able to solve the Green's function for this model "almost" analytically by going to normal modes:

$$Q_0 = \frac{1}{\sqrt{N}} \sum_{j=1}^N q_j \quad (17)$$

$$Q_i^{(c)} = \sqrt{\frac{2}{N}} \sum_{j=1}^N q_j \cos\left(\frac{2\pi i j}{N}\right) \quad i = 1, \dots, N/2 \quad (18)$$

$$Q_i^{(s)} = \sqrt{\frac{2}{N}} \sum_{j=1}^N q_j \sin\left(\frac{2\pi i j}{N}\right) \quad i = 1, \dots, N/2 - 1 \quad (19)$$

The prefactors are chosen so that the determinant of the coordinate transformation matrix is one. From now on the two indices of  $Q_i^{(c,s)}$  and  $P_i^{(c,s)}$  are merged to a single one which runs over all possible cases. In these new coordinates the Hamiltonian is separable:

$$H = P_0^2 + \sum_i \frac{\omega_i^2}{2} (Q_i)^2 = H_0 + \sum_i H_i \quad (20)$$

where

$$\omega_i = \sqrt{2 - 2 \cos \left( \frac{2\pi i}{N} \right)} \quad (21)$$

$H_0$  is the center of mass Hamiltonian, the  $H_i$  are related to the phonons. The Green's functions can then be decomposed:

$$\begin{aligned} G_t(Q_0 \dots Q_{N-1}; Q'_0 \dots Q'_{N-1}) &= \langle Q_0 \dots Q_{N-1} | e^{-i\hat{H}t} | Q'_0 \dots Q'_{N-1} \rangle \\ &= \langle Q_0 | e^{-i\hat{H}_0 t} | Q'_0 \rangle \prod_i \langle Q_i | e^{-i\hat{H}_i t} | Q'_i \rangle \\ &= G_t^{\text{Free}}(Q_0, Q'_0) \prod_i G_t^{\text{HO}}(Q_i, Q'_i) \end{aligned} \quad (22)$$

The corresponding operators satisfy the usual commutation relations:

$$[\hat{Q}_i, \hat{Q}_j] = [\hat{P}_i, \hat{P}_j] = 0 \quad (23)$$

$$[\hat{Q}_i, \hat{P}_j] = i\delta_{ij} \quad (24)$$

Due to the linearity of the transformation and the Jacobian being 1, one can show,

$$G_t(\vec{q}, \vec{q}') = G_t(\vec{Q}, \vec{Q}') \Big|_{\substack{\vec{Q}=\vec{Q}(\vec{q}) \\ \vec{Q}'=\vec{Q}'(\vec{q}')}} \quad (25)$$

in words, the Green's function in the original variables (needed in the integrations) is just given by the solved Green's functions in the new ones, with the new variables taking the values  $\vec{Q} = \vec{Q}(\vec{q})$ . The integration of Eq. (8) over the old  $q$  is over an „area” which is  $\mathbb{R}^{3N-3} \times I^2$  ( $I$  being the initial window). We performed these integrations numerically and chose  $N = 4$ . Particle number 1 was assumed to be for  $t = 0$  in the interval  $I = [-0.625; 0.625]$ . The probability density  $P(y_1, t = 0.5)$  was then calculated for two temperatures (see fig. 7). As expected, the higher temperature leads to a broader distribution, i.e. to a faster spreadening. Fig. 7 needed approximately 12 h of computing time on the vector processor of the RRZN in Hannover. Thus an increment in the number of particles would be possible only if one applies approximation techniques or performs some of the integrations analytically. It would be interesting in the future to study to which extent we have reached the thermodynamic limit in the sense that if

we have a very large circle of  $N$  oscillators the probability to find the first (or a close neighbour) in some position after some time, should not change when we go to  $N + 1$  oscillators. If this turns out to be the case we will have a good check on our formalism, as the rest of the degrees of freedom really form the heat bath and the theory is selfconsistently correct.

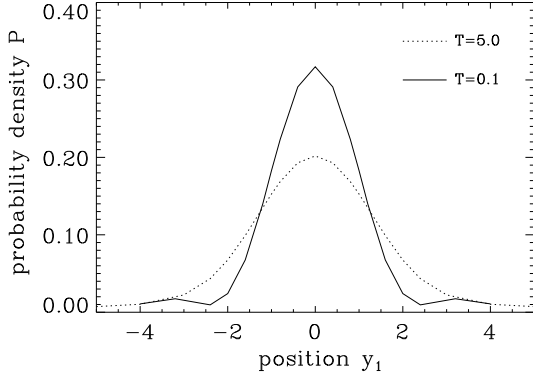


Figure 7: Probability to be at  $y$  for particle 1 of a ring of four particles, for time  $t = 0.5$ .

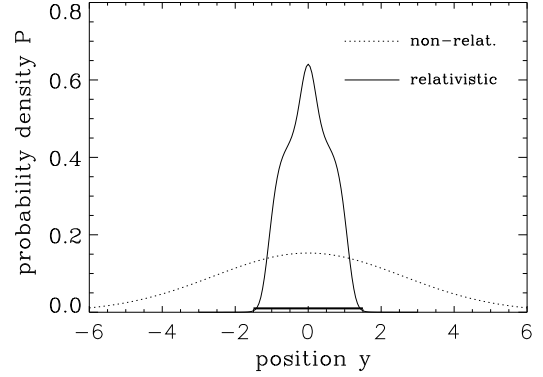


Figure 8: Comparison of the relativistic and non-relativistic free particle cases, with  $t=1$  and  $T=5$ .

#### 4.4 Relativistic Aspects

As can be extracted from the previous figures, the probability density broadens with speed  $v > c$  (we set  $c = 1$ ). This is no surprise, as we used ordinary non-relativistic Quantum Mechanics. To check if our correlation function can be extended to the relativistic regime, we chose the Hamiltonian

$$H_{\text{rel}} = \sqrt{p^2 + m^2}, \quad (26)$$

for a relativistic free particle. We had to use the FFT-method as only there the Hamiltonian formalism not yet integrated over momenta (instead of the Lagrangian) can be directly used. Fig. 8 compares the result with the free non-relativistic distribution. The horizontal bar is again the initial window, but it was switched on with an additional window function, taken as  $\exp(-3x^4)$ . The need for this smoothing is due to the well known problem of possible pair creation for relativistic fields, if a sharp rectangular window function is used. A high temperature was used to stimulate the fast dispersion due to high momenta modes. We can see that the relativistic wave packet is much more localized. An exponentially small violation of causality

can nevertheless be found here. The reason for it is that a fourier transform in a compact interval (the initial window) has necessarily components with negative frequencies (related to a small probability of pair creation), which cannot be included in our models in first quantization. Accordingly the small exponentially suppressed violation is entirely present immediately after the first measurement and does *not* increase with time as the probability broadens, as we have carefully checked for our system.

## 5 Conclusions

We have presented a formalism that describes real time evolution for some degrees of freedom in quantum systems at finite temperature. The description is necessarily of probabilistic nature as at finite  $T$  we are not in a pure state and one is not allowed to mix coherently amplitudes from different states in the thermal mixture. It is therefore doubtful if the usual time correlation function in thermal states will be directly checkable experimentally, unless we are close to the classical limit where  $H$  and  $\rho$  commute.

The probabilistic formalism for the time evolution can be expressed by a product of three Greens functions, one in Euclidean and two in real time, where one integrates over unobserved degrees of freedom. In the path integral formalism this corresponds to integrating over periodic paths in a complex time circuit, where we pinch the paths to the observed values (or ranges) at three (complex) times.

We presented various calculational methods to compute the required path integrals for complex time lines and showed that each one has its advantages, all converging eventually to the same answer. The matrix method is the fastest one, at least for low dimensional problems, requiring the highest memory resources. The FFT method needs less memory but takes a linear computing time with  $t$  or  $\beta = 1/T$ . The Monte Carlo method converges very slowly for real time propagation (no problem for large  $\beta$ ), but could still be used for very short time evolution, with least memory requirements. For all three methods it was useful to include a small imaginary  $\epsilon$  to the time propagation, which acts as an ultraviolet regulator.

We have first solved models with one degree of freedom in order to check the computational methods and gain confidence with this formalism, observing interesting phenomena as temperature dependence in the spreading probability, tunneling processes or near causality in the naive relativistic limit. The real consistency proof for our formalism should come in the thermodynamic limit of many degrees of freedom, in which we can assume that the initial quantum preparation of a small subset of the large quantum system will not bring the large system out of thermal equilibrium. Therefore, in this limit the probability density t-evolution should not change when we enlarge further the size of the system, the large quantum system providing the thermal bath for the correlation measurement. With the ring of  $N$  oscillators model, which we could solve analytically for the Greens functions, we were able to solve the needed integrations

over the spectator variables only up to 4 oscillators. This gave interesting results in its own right but we could not yet test the thermodynamic limit. Recently, a  $1 + 1$  dimensional Ising is being tested with this formalism [9], in order to check the thermodynamic limit. In this simplest field theory one only has two values for the spin at each site, making the problem computable with the matrix method. The transfer matrix has to be carefully tuned in its couplings in order to reach a continuum  $\Delta t \rightarrow 0$  limit. First results seem to confirm convergence of spin-correlation functions in time to limiting curves when one enlarges the spatial number of spins, thus indicating a thermodynamic limit. It remains to be seen if for more complicated field theories with interesting instanton effects, one can compute the real time pieces at least for short times for this formalism.

There are several aspects of this formalism still under study. For example the generalization from projector operators as observables, to more general operators. Also interesting is a better understanding of the linear response approximation starting from this formalism. Finally, one would like to have a better hold of the measurement process in quantum theories, to be included concretely into this formalism to study time evolutions.

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