Real-time correlation functions from imaginary-time evolution

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The problem of calculating real-time correlation functions is formulated in terms of an imaginary-time partial differential equation. The latter is solved analytically for the perturbed harmonic oscillator and compared with the known exact result. The first order approximation for the short-time propagator is derived and used for numerical solution of the equation by a Monte Carlo integration. In general, the method provides a reformulation of the dynamic sign problem, and is applicable to any two-time correlation function including single-particle, density-density, current-current, spin-spin, and others. The prospects of extending the technique onto multi-dimensional problems are discussed.

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I. INTRODUCTION

Quantum Monte Carlo (QMC) simulations proved very successful in studying many-body systems with realistic inter-particle potentials. Specific QMC methods have been developed for interacting electrons (for a recent review see [1]), liquid 4He [2], alkali Bose-condensates in harmonic traps [3], electron-proton plasma [4] and other systems. These methods yield accurate values of various physical properties, such as the cohesive energies of solids [5] or effective masses of defects [6], which are in excellent agreement with experiment. In model problems including spin [7], strong correlation [8], and electron-phonon [9,10] models, QMC usually handles much larger systems than other methods, treats equally well simple and complex interactions, and produces accurate results.

A major difficulty faced by QMC is its inability to compute reliably dynamic properties of quantum mechanical systems. This is because QMC operates in imaginary time. For those quantities that do not directly translate in an imaginary-time language, the simulation noise quickly exceeds the signal rendering the calculation impossible. This difficulty is known as the "dynamical sign problem". It is usually dealt with by computing correlation functions in imaginary time first, and then continuing the results into the real-time domain. For the latter step, Pade approximants [11], the maximum entropy [12], singular-value decomposition [13], and stochastic methods [14] are employed. Unfortunately, the analytic continuation of noisy data is an ill-posed mathematical procedure that does not lead to a unique solution. Sometimes such an uncertainty results in spectacular failures of the reconstruction strategy. For instance, even the most advanced and popular method, the maximum entropy, cannot resolve the two peaks of the dynamic structure factor in liquid helium [15]. This is a consequence of dealing with the mathematically ill-defined problem. Another difficulty is assigning meaningful error bars to the continuation procedure.

Thus the reconstruction procedure, while sometimes working reasonably well (especially in model systems), remain approximate, spoiling the rigor of QMC. What would improve the situation is the direct link between simulations and dynamic properties or rendering the problem mathematically well-posed. One such method was proposed by Mak and Egger who introduced "the multilevel blocking algorithm" to deal with the dynamic sign problem [16]. (A similar method was proposed for the fermion sign problem [17].) Essentially, this was an attempt of straightforward evaluation of real-time rapidly oscillating path integrals that express the time dependent transition amplitudes. This method requires very large computer memory even for simple one-particle systems. Since the sign problem becomes more severe with increasing the size of the system, the blocking algorithm may not sustain the increase in the number of simulated particles. It leaves the stimulus for the search of other alternatives.

In this paper, I propose another approach to alleviating the dynamic sign problem. The calculation of real-time correlators is formulated as a mathematically well-defined initial value problem for the operator $(\omega - H)^2$ which is of the fourth order in spatial coordinates. The solution of the corresponding imaginary-time evolution equation yields directly the frequency-dependent spectral function, thereby eliminating the need for the time Fourier transformation, analytic continuation and other intermediate procedures. The basic idea is very general and is applicable to any quantum mechanical system and any two-time correlation function. It is described in Section II. In Section III I apply the method to an exactly solvable case of disturbed one-dimensional harmonic oscillator. Solving the new equation in more general cases is hard and require stochastic Monte Carlo methods. The arising difficulties and their possible solutions are discussed in Sections IV-VII.
II. A DIFFERENTIAL EQUATION FOR THE SPECTRAL FUNCTION

Consider a typical problem of many-body physics, that of finding the single-particle zero-temperature correlator in an interacting $N$-particle system:

$$K(q,t) = \langle G | c_q(t) \hat{c}_q^\dagger(0) | G \rangle = e^{iHt} \langle G | c_q e^{-iHT} \hat{c}_q^\dagger | G \rangle.$$  \hspace{1cm} (1)

Here $|G\rangle$, $E_G$, and $H$ are the ground state, its energy, and the full Hamiltonian of the system, respectively. The particles could be either fermions or bosons. The operator $c_q^\dagger$ creates an extra particle with momentum $q$, and operator $c_q$ destroys it. It has to be emphasized that the single-particle momentum operators are chosen for definiteness only. In fact, everything that will be said and written about those operators will be equally valid for any pair of operators.] The notation $\hbar = 1$ is used throughout the paper. $K(q,t)$ describes the decay of $|\Psi(\omega) = c_q^\dagger |G\rangle$ with time due to $|\Psi\rangle$ not being an eigenstate of $H$. An equivalent amount of information is contained in the spectral density function $A(q, \omega)$ which is a Fourier transformation of $K(q,t)$:

$$A(q, \omega) = \int_{-\infty}^{\infty} K(q,t) e^{i\omega t} \text{d}t = (2\pi) \langle G | c_q \delta(\omega + E_G - H) \hat{c}_q^\dagger | G \rangle.$$  \hspace{1cm} (2)

Compare the structures of Eqs. (1) and (2). The correlation function is complex and has an oscillating kernel $e^{-iHT}$. The latter is the origin of the sign problem since big positive and negative contributions tend to cancel each other with a very small residue. On the contrary, $A(q, \omega)$ is positive definite and has a non-oscillating kernel, a delta-function, which intuitively makes it a better computational object. There is another, physical reason to prefer the function $A(q, \omega)$ over $K(q,t)$. The time-dependent properties themselves are rarely measured experimentally. What is usually inferred from experiments are namely the energy-dependent spectral functions, or related to them response functions. Thus rather than compute $K$s with subsequent numerical Fourier transformations, it would be much better to be able to compute $A$s directly. Besides, the main interest represent low-energy responses at small $\omega$s. This requires the knowledge of $K$s at large times $t$ that is precisely where the sign problem is worst.

The above considerations suggest to compute $A(q, \omega)$ instead of $K(q,t)$. \hspace{1cm} (3)

Taking the limit now amounts to solving the imaginary-time evolution equation

$$-\frac{\partial \psi}{\partial \alpha} = (\omega + E_G - H)^2 \psi,$$  \hspace{1cm} (4)

supplemented with the initial condition $\psi(\alpha = 0) = c_q^\dagger |G\rangle$.

The equation (1) and representation (3) are the main results of the paper. They show that dynamic correlators can in principle be obtained by solving an imaginary-time partial differential equation. The equation is supplemented by an initial condition and therefore it possesses a unique solution. The whole problem is thus mathematically well-defined. The full computational procedure is as follows: (i) Obtain a ground state wave function $|G\rangle$ and energy $E_G$ with whatever equilibrium method that works for the given system. (ii) Construct new state $|\Psi\rangle = c_q^\dagger |G\rangle$. (iii) Solve Eq. (1) using $|\Psi\rangle$ as an initial condition. (iv) Perform the $\alpha \rightarrow \infty$ limit and compute the scalar product with $|\Psi\rangle$ to get the spectral density for given frequency $\omega$. (v) Compute the response functions via fluctuation-dissipation and Kramers-Kronig relations.

Let me discuss the general properties of Eq. (1). First of all, this equation is of the first order in “time” variable $\alpha$ and fourth order in spatial coordinates because of the term $H^2$. Mathematically, this is a parabolic equation “correct in Petrovskii sense” \hspace{1cm} (4). Its properties are quite different from the familiar second order parabolic (diffusion) equations. In particular, its Green function is not positive-definite but instead can have positive and negative regions. Because of that, the proposed method does not solve the sign problem. Rather, it transforms the dynamic, or “time”, sign problem into a “space” sign problem which resembles the fermion one. More on this in Section (3). It is instructive to compare equation (1) with the imaginary time Schrödinger equation:

$$-\frac{\partial \psi}{\partial \beta} = (H - E_G)\psi.$$  \hspace{1cm} (5)

The latter’s formal solution $\psi(\beta) = e^{-\beta(H-E_G)}\psi(0)$. It shows that in the $\beta \rightarrow \infty$ limit, only the ground state survives because all the other states are exponentially suppressed. This well known fact is employed for instance in Projected Monte Carlo to extract the ground state out of an arbitrary initial state $\psi(0)$. The crucial observation here is that the energies of other states are all greater than $E_G$ which makes the exponent of the evolution operator be negative for all but the ground state. But what if one wants to retain not the
ground state but a state (or states) with energy \((E_G + \omega)\)? In this case one would need a similar evolution operator with the exponent being a negative and even function of \((E_G + \omega - H)\). The simplest function is quadratic one which results in precisely the exponential kernel of Eq. (3). Thus the physical meaning of the representation (4) is that in the course of evolution only excited states with excitation energy \(\omega\) survive and all the other states with excitation energies above and below \(\omega\) are exponentially suppressed. Notice also that while the variable \(\alpha\) in the Schrödinger equation is related to the inverse temperature, the variable \(\alpha\) in Eq. (4) has no clear physical meaning. The dimensionality of \(\alpha\) is \((\text{energy})^{-2}\). Lastly, one may think that many other variations of Eqs. (3) and (4) are possible since there are infinitely many limit representations of the delta-function. This does not seem to be the case. All other common representations of \(\delta(x)\) involve either non-analytical or non-polynomial functions (examples are \(e^{-\alpha|x|}\) and \(\alpha/(1 + x^2 \alpha^2)\)). Both cases make it difficult to interpret the resulting formulæ in terms of a simple evolution equation. Comparable or even better representations may exist but I could not find any.

I now rederive Eq. (4) differently, by demonstrating its equivalence to another definition of the spectral function. Let \(\phi_m\) be a set of eigenstates for the \((N+1)\)-particle system, \(H \phi_m = E_m \phi_m\). In general, \(|\Psi\rangle\) is not an eigenstate of \(H\) but it is always expandable in \(|\phi_m\rangle\):

\[
|\Psi\rangle = \sum_m a_m |\phi_m\rangle = \sum_m |\phi_m\rangle \langle \phi_m | c_q^\dagger | G\rangle. \tag{5}
\]

Upon substitution of the expansion in Eq. (3) the Hamiltonian in the exponent is replaced with \(E_m\). After that the \(\alpha \to \infty\) limit results in a delta-function \(\delta(\omega + E_G - E_m)\) and Eq. (3) becomes

\[
A(q, \omega) = (2\pi) \sum_m (G | c_q | \phi_m \rangle \langle \phi_m | c_q^\dagger | G\rangle) \delta(\omega + E_G - E_m), \tag{6}
\]

which is the usual definition of \(A(q, \omega)\) [3].

The formalism presented above is valid at zero temperature only. Its finite-temperature generalization is not straightforward and has to be addressed separately. The correlation function is defined as

\[
K(q, t) = \frac{1}{Z} \sum_n \langle n | e^{iHt} c_q e^{-iHt} c_q^\dagger e^{-\beta H} | n\rangle, \tag{7}
\]

where \(|n\rangle\) is a complete set of the \(N\)-particle system, \(\beta\) inverse temperature, and \(Z = \sum_n \exp(-\beta E_n)\) the partition function. A new difficulty in comparison with Eq. (3) is the second real-time operator \(e^{iHt}\) which acts in a different state space than \(e^{-iHt}\). Therefore, a time Fourier transform of Eq. (3) does not lead to a convenient representation of the spectral density similar to Eq. (4). Put differently, \(e^{-iHt}\) cannot be replaced with a \(c\)-number because it now acts not on a single state but on the whole set \(|n\rangle\) which is not supposed to be known in its entirety. Still, one can proceed further by formally separating the time variables in the two operators. Introducing an auxiliary delta-function \(1 = \int dt' \delta(t - t')\), replacing \(t \to t'\) in \(e^{-iHt}\), using \(\delta(t - t') = \int \frac{d\omega}{2\pi} e^{-i\omega(t - t')}\), and integrating over \(t'\) one obtains

\[
K(q, t) = \frac{1}{Z} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \sum_n \langle n | e^{iHt} c_q \delta(\omega - H) c_q^\dagger e^{-\beta H} | n\rangle. \tag{8}
\]

A Fourier transformation yields for the spectral density

\[
A(q, \omega) = \frac{2\pi}{Z} \int_{-\infty}^{\infty} d\omega \sum_n \langle n | \delta(\omega - \varepsilon + H) c_q \delta(\omega - H) c_q^\dagger e^{-\beta H} | n\rangle
\]

\[
= \frac{2\pi}{Z} \lim_{\omega_1 \to -\infty} \lim_{\omega_2 \to \infty} \int_{-\infty}^{\infty} d\omega \sum_n \langle n | e^{-\alpha_1 (\omega - \varepsilon + H)^2} c_q e^{-\alpha_2 (\omega - H)^2} c_q^\dagger e^{-\beta H} | n\rangle. \tag{9}
\]

There are three imaginary-time evolution processes in the last equation. First one, starting with an arbitrary state \(|n\rangle\), during time \(\beta\), and under operator \(H\). Second one, starting from the finite state of the first process plus an extra particle with momentum \(q\), during infinite time, and under operator \((\varepsilon - H)^2\). Third one, starting with the final state of the second process minus a particle with momentum \(q\), during infinite time, and under operator \((\omega - \varepsilon + H)^2\). In the end, the scalar product with \(|n\rangle\) and integration over the real variable \(\varepsilon\) have to be done. In the zero-temperature limit, the operator \(e^{-\beta H}\) projects out all but the ground states, \(e^{-\beta H} | n\rangle = e^{-\beta E_G} | G\rangle \delta_{nG}\), and then the factor \(e^{-\beta E_G}\) cancels \(Z\). After that, the leftmost \(H\) in Eq. (3) is replaced with \(E_G\) and the limit in \(\alpha_1\) and integration over \(\varepsilon\) are easily performed, thereby reducing Eq. (4) to the previous expression (3).

The finite-temperature generalization is achieved at the expense of the second auxiliary evolution and an extra integration. This makes any practical realization of the method much more difficult than at zero temperature. Nevertheless, Eq. (4) is exact and contains only real exponentials.

In conclusion of this section, let me reiterate that nowhere the specifics of the single particle operators (fermionic or bosonic) have been used. Everything that has been said about \(c_q\) and \(c_q^\dagger\) is equally applicable to any pair of operators \(\hat{O}_1\) and \(\hat{O}_2\). A generic expression for the zero-temperature spectral density is a straightforward generalization of Eq. (4):

\[
A_{\hat{O}_1 \hat{O}_2}(\omega) = (2\pi) \lim_{\alpha \to \infty} \langle G | \hat{O}_2 \sqrt{\frac{\alpha}{\pi}} e^{-\alpha(\omega + E_G - H)^2} \hat{O}_1 | G\rangle. \tag{10}
\]
There are no restrictions on the choice of the operators $\hat{O}_1$ and $\hat{O}_2$. They could be single-particle, two-particle, spin, or other. In the case of the density or current operators, Eq. (11) opens the exciting possibility to compute dynamic structure factors and conductivities from first principles.

III. PERTURBED HARMONIC OSCILLATOR: ANALYTICAL SOLUTION

The purpose of this Section is to solve a non-trivial example to demonstrate Eqs. (12) and (13) at work. Consider a harmonic oscillator with frequency $\Omega$ and mass $M$. It can be either free of subjected to a constant force of magnitude $g\sqrt{2M}\hbar\Omega^2$, depending on whether an additional particle is present in the vicinity of the oscillator or not. The Hamiltonian reads

$$H_x = \Omega \left( -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} x^2 - \sqrt{2} gx e^{\dagger} c \right),$$

where the coordinate $x$ is measured in units of $\sqrt{\hbar/(M\Omega)}$ and $g$ is the dimensionless coupling constant. This Hamiltonian is known from the independent boson model [18]. It can also be thought of as the on-site Holstein polaron [20]. Let the oscillator be in its ground state and the particle absent at $t < 0$. The state of the system is $|G\rangle = |0_{\text{part}},0_x\rangle = |0_{\text{part}},\frac{1}{\sqrt{2}} e^{-x^2/2}\rangle$ with energy $E_G = \frac{1}{4}\Omega$. At time 0 the particle is placed on the oscillator creating state $|\psi(x,\alpha = 0)\rangle = |1_{\text{part}},0_x\rangle$. At this time the oscillator begins to experience the force. At time $t$ the particle is removed and the oscillator is left free but in one of the excited states $|m_x\rangle$. So between 0 and $t$ the Hamiltonian is

$$H_x = \Omega \left( -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} x^2 - \sqrt{2} gx \right).$$

Our objective is to compute the spectral function $A(\omega)$ of operators $c\dagger$ and $c$. According to the general scheme, one requires to solve equation (11) with $H_x$ from (12) and initial condition $|0_x\rangle$. This can be done by introducing first a new variable $y = x - \sqrt{2} g$, and then bosonic operators $b_y$ and $b_y\dagger$. The transformed Hamiltonian is $H_y = \Omega(b_y\dagger b_y - g^2 + \frac{1}{4})$. After expansion of the solution in the eigenstates of $b_y\dagger b_y$, $|\psi\rangle = \sum_{m=0}^{\infty} a_m(\alpha)|m_y\rangle$, Eq. (12) becomes:

$$-\sum_{m=0}^{\infty} \frac{\partial a_m(\alpha)}{\partial \alpha} |m_y\rangle = \sum_{m=0}^{\infty} a_m(\alpha)(\omega + g^2\Omega - \Omega b_y\dagger b_y)^2 |m_y\rangle
= \sum_{m=0}^{\infty} a_m(\alpha)(\omega + g^2\Omega - \Omega m)^2 |m_y\rangle. \quad (13)$$

Equations with different $m$ are separated and easily integrated yielding

\begin{align*}
\psi(x,\alpha) &= \sum_{m=0}^{\infty} a_m(0)e^{-\alpha(\omega + g^2\Omega - \Omega m)^2} \\
&\quad \times \frac{1}{\sqrt{2}\sqrt{2m}} H_m(x - \sqrt{2} g)e^{-\frac{1}{2}(x - \sqrt{2} g)^2}, \quad (14)
\end{align*}

where $H_m(x)$ are the Hermite polynomials. The coefficients $a_m(0)$ are found from the initial condition $\psi(x,0) = e^{-x^2/2}$:

$$a_m(0) = \langle m_y|0_x\rangle = (\frac{\sqrt{2} g}{\sqrt{2m!}})^m e^{-\frac{1}{2}g^2}. \quad (15)$$

Figure 1 shows the solution (14)-(15) at different “times” $\alpha$. $g = 1.5$ and $\omega = 2.0\Omega$. Note how negative pockets develop with time. After $\alpha = 5.0$ the solution changes only slightly.

$$A(\omega,\alpha) = (2\pi)e^{-g^2} \sum_{m=0}^{\infty} \frac{g^{2m}}{m!} \sqrt{\frac{2}{\pi}} e^{-\alpha(\omega + g^2\Omega - \Omega m)^2}. \quad (16)$$

Figure 2 illustrates the changes in $A(\omega,\alpha)$ as $\alpha$ progresses from 0 to $\infty$. The solution evolves from the identical zero through a smooth single peak to a highly non-analytical grid of delta-functions. The $\alpha \to \infty$ limit of Eq. (16) results in

$$A(\omega) = (2\pi)e^{-g^2} \sum_{m=0}^{\infty} \frac{g^{2m}}{m!} \delta(\omega + g^2\Omega - \Omega m), \quad (17)$$

which is known to be the correct spectral density [18] (chapter 4).

Two comments are appropriate at this point. The first one concerns the solvability of the equation (11). In the above example, the equation was solvable because the oscillator before, during, and after the perturbation was an

![Figure 1](image1.png)

![Figure 2](image2.png)
FIG. 2. The spectral function of the perturbed harmonic oscillator for different values of the parameter \( \alpha \). The first (leftmost) peak appears at \( \omega = -g^2\Omega \). The area under all the curves is \( 2\pi \). This is how the correct result would emerge in the course of numerical solution of Eqs. (14) and (16).

Integrable system in which eigenfunctions were well known. Surely, for any such a system where all the eigenfunctions are known, the equation would be solvable as easily as for the oscillator, and the results would be expressible in the form of a spectral expansion similar to Eqs. (14)-(16).

The second observation is about the differences between systems with discrete and continuous spectrum. In the case of discrete spectrum, as in the above example, the equation would be solvable as easily as for an integrable system which eigenfunctions were well known. For systems with discrete spectrum, including all real systems, the overlap function for these resonant frequencies. For systems with harmonic oscillator for different values of the parameter \( \alpha \) in the limit \( \alpha \rightarrow \infty \), then the factor \( \sqrt{\alpha} \) results in infinite limit values of the spectral function for these resonant frequencies. For systems with continuous spectra, including all real systems, the overlap and consequently the solution of the Green’s function (GF) of the evolution operator:

\[
G(X', X; \alpha, \varepsilon) = \langle X' | e^{-\alpha(\varepsilon-H)^2} | X \rangle, \\
\]

where \( X = \{x_i\} \) and \( X' = \{x_i'\} \) are two sets of the system’s coordinates. The number of coordinates is \( n = Nd \), \( N \) being the number of particles and \( d \) the dimensionality of space. I have also used the notation \( \varepsilon \) to represent the sum \( \omega + E_G \). Let us find GF for the system of free distinguishable particles with unit mass which is described by Hamiltonian

\[
H_0 = \hat{T} \equiv -\frac{1}{2} \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2} = \frac{1}{2} \nabla_n^2, \\
\]

where \( \nabla_n \) is the \( n \)-dimensional gradient operator. Introducing the momentum states \( |K\rangle \) via

\[
|X\rangle = \int_{-\infty}^{\infty} \frac{dK}{(2\pi)^n} e^{iKX}|K\rangle, \\
\]

and using \( \langle K' | K \rangle = (2\pi)^n \delta(K - K') \) one obtains from (13)

\[
G_0(X', X; \alpha, \varepsilon) = \int_{-\infty}^{\infty} \frac{dK}{(2\pi)^n} e^{iK(X-X')} e^{-\alpha(\varepsilon - \frac{K^2}{2})^2}. \\
\]

The last expression satisfy the initial condition \( G_0(X', X; \alpha = 0) = \delta(X - X') \). As expected from the translational invariance, GF is a function of the difference \( X - X' \). The rotational invariance of space also suggests that GF must be the function of the modulus \( |X - X'| \equiv R \) only. This is indeed the case which allows the reduction of Eq. (21) to a one-dimensional integral (technical details are not important for the purposes of this paper):

\[
G_0(R; \alpha, \varepsilon) = \frac{2\pi^{\frac{n}{2}}}{(2\pi)^n} \int_0^\infty dk k^{n-1} \frac{J_{n-1}(kR)}{(2\pi)^{\frac{n}{2}-1}} e^{-\alpha(\varepsilon - \frac{k^2}{2})^2}, \\
\]

where \( J_{n-1}(x) \) is the Bessel function. In one dimension, \( n = 1 \), it follows from Eq. (22) or directly from Eq. (21) that

\[
G_0(x, x; \alpha, \varepsilon) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \cos[k(x - x')] e^{-\alpha(\varepsilon - \frac{k^2}{2})^2}. \\
\]

The last equation is a convenient place to compare the properties of the imaginary time Schrödinger equation (or diffusion equation) with those of Eq. (16). In the former case, the corresponding expression for \( G_0^{n=1} \) would have just \( k \) in place of \( \varepsilon - \frac{k^2}{2} \). Then, the integral would easily be performed leading to the positive-definite GF of the diffusion equation. In the present case, despite the integral cannot be performed analytically, it is easy to see that GF is not positive definite. Indeed, take the limit of large \( \alpha \). The integral is dominated by the points...
\[ G(x', x; \alpha, \epsilon) = \int dX_1 \ldots dX_L G(x', X_L; \Delta \alpha) \ldots G(X_1, X; \Delta \alpha). \] (25)

The number of additional time slices \( L \) must be chosen large so that the new time interval \( \Delta \alpha = \frac{\alpha}{L+1} \) gets small enough to allow accurate approximations of \( G(X_{i+1}, X_i; \Delta \alpha) \). The main difficulty in constructing those approximations is the non-commutativity of the kinetic and potential operators \( T \) and \( \hat{V} \). This difficulty is usually overcome by the Trotter-Suzuki decomposition of exponential operators, see, e.g., [22]. However, in the present case one is faced with a completely new situation. The exponent of the evolution operator [the right-hand side of Eq. (9)] contains not only sums but also products of non-commuting operators, namely \( \hat{T} \hat{V} \). Thus all the reciprocities have to be devised anew. In the first order in \( \Delta \alpha \) it can be done in the following way. Expand the exponential in Eq. (18):

\[ G(X_{i+1}, X_i; \Delta \alpha, \epsilon) = \langle X_{i+1} \left\{ 1 - \Delta \alpha (\epsilon - \hat{T} - \hat{V}) (\epsilon - \hat{T} - \hat{V}) + o(\Delta \alpha) \right\} | X_i \rangle. \] (26)

In the term linear in \( \Delta \alpha \), the potential operator in the first parantheses can be replaced with its value at the final configuration: \( \hat{V} \rightarrow V(X_{i+1}) = V_{i+1} \). Similarly, the potential operator in the second parantheses can be replaced with its value at the initial configuration: \( \hat{V} \rightarrow V(X_i) = V_i \). Exponentiating back, one obtains

\[ G (X_{i+1}, X_i; \Delta \alpha, \epsilon) \approx \langle X_{i+1} | e^{-\Delta \alpha (\epsilon - V_{i+1} - \hat{T}) (\epsilon - V_i - \hat{T})} | X_i \rangle \]

\[ = e^{\frac{\Delta \alpha}{2} (V_{i+1} - V_i)^2} \langle X_{i+1} | e^{-\Delta \alpha \left[ \frac{1}{2} (V_{i+1} + V_i) - \hat{T} \right]^2} | X_i \rangle \]

\[ = e^{\frac{\Delta \alpha}{2} (V_{i+1} - V_i)^2} G_0 \left( X_{i+1}, X_i; \Delta \alpha, \epsilon - \frac{1}{2} (V_{i+1} + V_i) \right). \] (27)

The last line expresses the short-time propagator of the interacting system via the short-time propagator of the non-interacting system \( G_0 \) taken at a shifted energy argument. This result together with Eq. (22) lead to the following remarkable conclusion: even in a many-body interacting system calculation of the short-time propagator requires knowledge of the potential energy at the end points and only one one-dimensional integration. Moreover, since the integral in Eq. (22) is a universal function for given \( n \) and \( \alpha \), it can be easily tabulated for all required values of \( \epsilon \) and \( |X_{i+1} - X_i| \).

Of fundamental importance is the question whether the higher order approximations could be derived. Preliminary studies suggest a positive answer albeit with much more cumbersome expressions than Eq. (27). Continuing the expansion in Eq. (26) further one finds in the next term already four factors \( \epsilon - \hat{T} - \hat{V} \). Only two operators \( \hat{V} \) can be replaced with numbers immediately, the other two have to be commuted through \( \hat{T} \)s. Such
a process generates multiple additional terms that contain \((\nabla_n V)s\) and \((\nabla_n^2 V)s\). I do not show specific details here but it is clear that the second order approximation would be much harder to evaluate numerically than the first order one, especially in the multi-dimensional situation. Obviously, a special study is needed to investigate whether such a complexity is worth the gained accuracy and the consequent increase of the time step \(\Delta \alpha\).

V. INTEGRATION

With the short-time propagator known for given excitation energy \(\omega\) and time step \(\Delta \alpha\), the \(\alpha\)-dependent spectral function" is given by the multiple integral

\[
A(\alpha) = (2\pi) \sqrt{\frac{\alpha}{\pi}} \int_0^\infty dX_1 \ldots dX_L dX' \times \\
\Phi(X') G(X', X_1; \Delta \alpha) \ldots G(X_1, X; \Delta \alpha) \Psi(X),
\]

where \(\Psi\) and \(\Phi\) are the initial and final states of the system. (Recall that \(\Psi\) and \(\Phi\) may not be the same, this depends upon the choice of the operators \(O_1\) and \(O_2\) studied.) While trying to evaluate the above integral one faces an immediate difficulty of infinite limits of integration. It can be resolved by introducing auxiliary normalized probability densities \(P(X)\) with properties \(P(X) > 0\) and \(\int dXP(X) = 1\). Then the last equation is rewritten identically as follows

\[
A(\alpha) = \sqrt{\frac{\alpha}{\pi}} \int dX_1 \ldots dX' W P'(X') \ldots P_1(X_1) P(X)
\]

\[
(29)
\]

\[
W \equiv \frac{\Phi(X') G(X', X_1; \Delta \alpha) \ldots G(X_1, X; \Delta \alpha) \Psi(X)}{P'(X') P_1(X_1) \ldots P_1(X_1) P(X)}
\]

\[
(30)
\]

As a result of this transformation, the product of functions \(P\) can serve as the weight function. The explicit form of functions \(P\) is completely at our disposal. It should be chosen to minimize the probability of large deviations of \(Xs\). The functions \(P\) need not be all the same. Each \(P\) is absolutely arbitrary and independent of the other as long as the main conditions of positivity and normalization are fulfilled. In short, functions \(P\) serve to optimize stochastic integration of Eq. (29).

![Image](image-url)

FIG. 4. The Green function (31) for \(\alpha = 2.0 \Omega^{-2}\) and \(\omega = -2.75 \Omega\) (top left), \(\omega = -1.75 \Omega\) (top right), \(\omega = -0.25 \Omega\) (bottom left), and \(\omega = 1.25 \Omega\) (bottom right). The number of nodes increases with excitation energy. The two horizontal axes are \(x\) and \(x'\).

Note also that the absolute values of the Green’s functions \(|G|\) cannot be used as auxiliary probability densities because their normalization is not known a priori. One may think that one could get away from this obstacle by simply assuming some normalization factor and then restoring it afterwards from the overall normalization of the spectral function. While this can work in principle, this would require a very accurate determination of \(A\)

\[
G(x', x; \alpha, \omega) = \frac{1}{\sqrt{\pi}} e^{-\frac{1}{2} (x' - \sqrt{2 g})^2} e^{-\frac{1}{2} (x - \sqrt{2 g})^2} \times
\]

\[
\sum_{m=0}^\infty \frac{1}{2m!} H_m(x' - \sqrt{2 g}) H_m(x - \sqrt{2 g}) e^{-\alpha (\omega + g^2 \Omega - \Omega m)^2}
\]

\[
(31)
\]

This function is shown in Figure 4 for \(\alpha = 2.0 \Omega^{-2}\) and several excitation energies \(\omega\). Notice how the number of sign changes increases with \(\omega\). An analogy seems to exist between this fact and the increase in the number of nodes of the eigenstates of the time-independent Schrödinger equation.

One can use the exact solution (31) to check the accuracy of the approximate representation (27). Due to
the one-dimensional character of the problem the check can be very effectively done as follows. The approximate short-time propagator is computed for some small time step \( \Delta \alpha \). Then the propagator corresponding to the double time \( G(2\Delta \alpha) \) is found by convolving two \( G(\Delta \alpha) \)'s. If \( G(x', x; \alpha) \)'s are represented by matrices with matrix elements evaluated on a uniform mesh \( (x'_i, x_j) \) then the convolution is equivalent to squaring of matrix \( G(x', x_j; \Delta \alpha) \equiv G_{ij}(\Delta \alpha) \):

\[
\hat{G}_{ij}(2\Delta \alpha) = \Delta x \hat{G}_{ij}^2(\Delta \alpha),
\]

where \( \Delta x \) is the step of the coordinate mesh. Repeating the squaring \( n \) times one arrives at the propagator corresponding to the large time interval \( 2^n \Delta \alpha \), which is compared with the exact result. In this manner it was established that the rule \( \hat{G}_{ij} \) is not as accurate as the one without the exponential factor \( \exp[\frac{\Delta \alpha}{\Omega} (V_{i+1} - V_i)^2] \). For instance, at \( \Delta \alpha = 0.05 \Omega^{-2} \) the expression without the factor remains within 10% from the exact solution even after 9 squaring which corresponds to 512 time steps or total time \( \alpha = 25.6 \Omega^{-2} \), in a wide range of energies \(-2.75 < \omega/\Omega < 2.75\). At the same time, the formula with the exponential factor demonstrated deviations \( \sim 100\% \) already at 7 squaring, i.e., at times \( \alpha \approx 0.4 \Omega^{-2} \). At larger \( \Delta \alpha \approx 0.2 - 0.4 \Omega^{-2} \), both versions were bad, Eq. \( \hat{G}_{ij} \) overestimating the one without the factor underestimating the correct values of the long-time propagator. The best results were obtained with the factor but with the coefficient in the exponent being \( \approx 0.10 \) instead of 0.25 as in Eq. \( \hat{G}_{ij} \).

It is not the purpose of the paper to perform a detailed examination of this issue. Given the complex character of the new evolution operator, a complete analysis could be quite involved. A possible reason for the described inconsistency may be a bigger than expected role of the higher-order terms neglected in deriving approximation \( \hat{G}_{ij} \). A better understanding of this role requires explicit derivation of the second and possibly third-order approximations and their thorough comparison. This is a difficult task that warrants a separate study.

Let me now present the results of numerical integration of Eqs. \( \hat{G}_{ij} \). I have used gaussian functions \( P(x) \) and the simplest “brute force” method of integration when uncorrelated sequence of configurations \( \{x\} \) is generated and the quantity \( W \) measured and accumulated in a straightforward manner. A crucial parameter in the process is the number of time intervals or the total number of integrations. As long as the number of integrations is less than about 20 the sign problem does not manifest itself and the simulations produce accurate results with controllable error bars. An example is shown in Figure 5 where the exact propagator \( \hat{G}_{ij} \) is used. The multipeak structure of the spectral function is clearly resolved. Similar encouraging results have been obtained for other time steps and number of steps, for instance
The number of measurements is 17. (This is the reason for larger error bars as compared with Figure 5.) The number of integrations is required. An example considered in Section VI demonstrates of its viability. Thirdly, and perhaps most importantly, the “brute force” method of integration is not the right way to solve the equation (4). The incredible progress of Monte Carlo methods in the past decades has been largely due to the “smart” ways of performing multiple integrations such as the Metropolis algorithm in statistical applications or the importance sampling in fermionic applications. In relation to the present paper, the recent exact fermionic algorithm of Kalos and Ped- eriva [23] looks particularly interesting. They developed a Diffusion Monte Carlo algorithm for finding the ground state of the many-body fermionic Schrödinger equation with no approximation. Their method can handle wave functions with positive and negative regions, so it effectively solves the fermionic sign problem. Precisely an algorithm of this kind is required for solving equation (4). It is too early to judge whether these ideas could be directly applied here but this is definitely one of possible directions to search for an effective method of integration.

less may have simpler structure functions. There is not much sense in perfecting the solution when there is no guarantee that the tricks developed will work in the physically more interesting cases. The results given above serve primarily as an illustration to the method and a demonstration of its viability. Thirdly, and perhaps most importantly, the “brute force” method of integration is not the right way to solve the equation (4). The incredible progress of Monte Carlo methods in the past decades has been largely due to the “smart” ways of performing multiple integrations such as the Metropolis algorithm in statistical applications or the importance sampling in fermionic applications. In relation to the present paper, the recent exact fermionic algorithm of Kalos and Ped- eriva [23] looks particularly interesting. They developed a Diffusion Monte Carlo algorithm for finding the ground state of the many-body fermionic Schrödinger equation with no approximation. Their method can handle wave functions with positive and negative regions, so it effectively solves the fermionic sign problem. Precisely an algorithm of this kind is required for solving equation (4). It is too early to judge whether these ideas could be directly applied here but this is definitely one of possible directions to search for an effective method of integration.

VII. CONCLUSIONS

This paper describes a novel approach to direct stochastic calculation of dynamic correlation functions of quantum mechanical systems. It was inspired by the difficulties of the traditional reconstruction methods originating from the absence of a mathematically rigorous formulation of the analytical continuation procedure. I believe that at present the quest for an effective way of computing the dynamic correlators directly in real time/frequency domain is fully justified, and it should continue until any of the two approaches results in an effective and satisfactory numerical algorithm.

Let me summarize how the present paper contributes to this process. It has been proposed to make the spectral function \(A(\omega)\) rather than the time-dependent correlator \(K(t)\), the main object of the computational effort. This is advantageous because it directly leads to experimentally accessible properties and avoids the need for additional procedures such as Fourier transformations. The calculation of the spectral function is made possible by replacing the operator delta-function with the limit of a gaussian and by interpreting the latter as a long-time solution of the evolution equation (4). Thus the process of finding \(A(\omega)\) is formulated as an initial value problem for a fourth-order differential operator. Such a problem is mathematically well-defined and has a unique solution. One “only” requires to solve the equation in the limit of infinite time \(\alpha\). The solutions can be classified with respect to their limit behavior. Some will remain constant which will lead to infinite values of the spectral function (apparently at discrete energies only). Other solutions should decay as \(1/\sqrt{\omega}\) and lead to finite \(A(\omega)\). Third class comprises solutions decaying faster than that (probably exponentially) and resulting in vanishing \(A(\omega)\). In the end, taking a scalar product with a function of interest is required. The whole sequence should be repeated for all relevant excitation energies. The new formulation has been shown to be equivalent to the standard theory and definitions of the spectral function. It has also been generalized to finite temperatures. Another positive feature of the method is its universality. It imposes absolutely no restrictions on the nature of the operators studied. They could be bosonic or fermionic, one-particle, two-particle, or even more complex, current, density, spin, and so on. Also the spectral functions are not required to possess any special properties such as non-negativity, additional symmetries, and sum rules. In short, the theory is simple, mathematically well-defined, and universal.

The practical usefulness of the proposed method will be very much dependent on the availability of stochastic methods that could solve equation (4) in multi-dimensional cases. Since the propagator necessarily has negative regions, handling of sign-alternating functions is required. An example considered in Section VII demon-
strates that this is achievable. In broader terms, the situation bears strong similarities with Diffusion Monte Carlo studies of systems of interacting fermions, where a significant progress was reported \[23,24\]. Additional work is needed to develop similar approaches for equation (4). If successful, the effort will bring direct ways of first-principle Monte Carlo studies of dynamic characteristics of quantum mechanical systems.

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