Efficient Quantum Algorithm for Computing $n$-time Correlation Functions

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We propose a method for computing $n$-time correlation functions of arbitrary spinorial, fermionic, and bosonic operators, consisting of an efficient quantum algorithm that encodes these correlations in an initially added ancillary qubit for probe and control tasks. For spinorial and fermionic systems, the reconstruction of arbitrary $n$-time correlation functions requires the measurement of two ancilla observables, while for bosonic variables time derivatives of the same observables are needed. Finally, we provide examples applicable to different quantum platforms in the frame of the linear response theory.

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Quantum mechanics is a a recipe for computing probability distributions of measurement outcomes in given experiments, typically, at the microscopic scale [1]. Developed since the early years of the twentieth century, quantum mechanics has allowed us to describe the most fundamental properties of light and matter, such as quantum superposition and entanglement [2], or the behavior of elementary particles emerging from scattering processes [3]. More recently, with the advent of modern quantum technologies [4–7], quantum mechanics has become the roadmap for the design of computational protocols and simulations of physical systems beyond the capabilities of classical devices [8, 9]. In this renewed view, proof-of-principle experiments have implemented quantum simulations with the promise of an exponential speedup in the information processing [10–16].

According to quantum theory, all information about a system, its stationary states and evolution, is encoded in the Hamiltonian. Nonetheless, for most cases, the extraction of this information may not be straightforward [17, 18]. Therefore, alternative strategies are needed to identify and obtain measurable quantities that characterize the relevant physical information [19]. A case of particular importance is given by response functions and susceptibilities, which in the linear response theory are computed in terms of two-time correlation functions [20–22]. In this sense, for example, the knowledge of two-time correlation functions of the form $\langle \Psi | A(t) B(0) | \Psi \rangle$, stemming from perturbation theory, provides us with a microscopic derivation of useful quantities as conductivity and magnetization [23]. The reconstruction of time-correlation functions, however, need not be trivial at all, and could profit from quantum algorithm and simulation protocols for their determination. The computation of time correlation functions for propagating signals is at the heart of quantum optical methods [24], including the case of propagating quantum microwaves [25–27]. However, these methods are not necessarily easy to export to the case of spinorial, fermionic and bosonic degrees of freedom of massive particles. In this sense, recent methods have been proposed for the case of two-time correlation functions associated to specific dynamics in optical lattices [28], as well as in setups where post-selection and cloning methods are available [29].

Let us thus consider a two-time correlation function $\langle A(t) B(0) \rangle$ where $A(t) = U^\dagger(t) A(0) U(t)$, $U(t)$ being a given unitary operator, while $A(0)$ and $B(0)$ are both Hermitian. Remark that, generically, $A(t) B(0)$ will not be Hermitian. However, one can always construct two self-adjoint operators $C(t) = \frac{1}{2} \{ A(t), B(0) \}$ and $D(t) = \frac{1}{2} [ A(t), B(0) ]$ such that $\langle A(t) B(0) \rangle = \langle C(t) \rangle + i \langle D(t) \rangle$. According to the quantum mechanical postulates, there exist two measurement apparatus associated with observables $C(t)$ and $D(t)$. In this way, we may formally compute $\langle A(t) B(0) \rangle$ from the measured $\langle C(t) \rangle$ and $\langle D(t) \rangle$. However, the determination of $\langle C(t) \rangle$ and $\langle D(t) \rangle$ depends non trivially on the correlation times and on the complexity of the specific time evolution operator $U(t)$. Furthermore, we point out that the computation of $n$-time correlations, as $\langle \Psi | \Psi ' \rangle = \langle \Psi | U(t) A U(t) B | \Psi ' \rangle$, is not a trivial task even if one has access to full state tomography, due to the ambiguity of the global phase of state $| \Psi ' \rangle = U(t) A U(t) B | \Psi \rangle$. Therefore, we are confronted with a cumbersome problem: the design of measurement apparatus depending on the system evolution for determining $n$-time correlations of a system whose evolution may not be accessible. To our knowledge, a general formalism to attack this problem is still missing, while alternative algorithmic strategies [30] may be considered.

In this Letter, we propose an efficient quantum algorithm for computing general $n$-time correlation functions of an arbitrary quantum system, requiring only an initially added probe and control qubit. Moreover, our method is applicable to a general class of interacting spinorial, bosonic, and fermionic systems. Finally, we provide examples of our protocol in the frame of the linear response theory, where $n$-time correlation functions are needed.

Assume that we are provided with a controllable quantum system undergoing a given quantum evolution described by the Schrödinger equation

$$i \hbar \partial_t | \phi \rangle = H | \phi \rangle.$$  

(1)

We are going to design a protocol for the efficient measurement of generalized $n$-time correlation functions of the form $\langle \phi | \theta_{n-1} (t_{n-1}) \theta_{n-2} (t_{n-2}) \cdots \theta_1 (t_1) \theta_0 (t_0) | \phi \rangle$, where...
\( \theta_{n-1}(t_{n-1})...\theta_0(t_0) \) are certain operators evaluated at different times, e.g. \( \theta_k(t_k) = U(1)(t_k; t_0)\theta_0(t_k), \) \( U(1)(t_k; t_0) \) being the unitary operator evolving the system from \( t_0 \) to \( t_k \). For the case of dynamics governed by time-independent Hamiltonians, \( U(t_k; t_0) = U(t_k - t_0) = e^{-\frac{i}{\hbar}H(t_k - t_0)} \). However, our method applies also to the case where \( H = H(t) \), and can be sketched as follows. First, the ancillary qubit is prepared in state \( \frac{1}{\sqrt{2}}(|\psi| + |g|) \) with \( |g\rangle \) its ground state, as in step 1 of Fig. 1, so that the whole ancilla-system quantum state is \( \frac{1}{\sqrt{2}}(|\psi| + |g|) \otimes |\phi\rangle \), where \( |\phi\rangle \) is the state of the system. Second, we apply the controlled quantum gate \( U_c^0 = \exp\left(-\frac{i}{\hbar}|g\rangle\langle g| \otimes H_0 \tau_0\right) \), where, as we will see below, \( H_0 \) is a Hamiltonian related to the operator \( \theta_0 \), and \( \tau_0 \) is the gate time. As we point out later, this entangling gate can be implemented efficiently with two Mølmer-Sørensen gates for operators \( \theta_0 \) that consist in a tensor product of Pauli matrices [31]. This operation entangles the ancilla with the system generating the state \( \frac{1}{\sqrt{2}}(|\psi| \otimes |\phi\rangle + |g\rangle \otimes \tilde{U}_c^0|\phi\rangle) \), with \( \tilde{U}_c^0 = e^{-\frac{i}{\hbar}H_0 \tau_0} \), step 2 in Fig. 1. Next, we switch on the dynamics of the system governed by Eq. (1). For the sake of simplicity let us assume \( t_0 = 0 \). The effect on the ancilla-system wavefunction is to produce the state \( \frac{1}{\sqrt{2}}(|e\rangle \otimes U(t_1; t_0)|\phi\rangle + |g\rangle \otimes \tilde{U}_c^0|\phi\rangle) \), step 3 in Fig. 1. Note that, remarkably, this last step does not require an interaction between the system and the ancillary-qubit degrees of freedom nor any knowledge of the Hamiltonian \( H \). These techniques, as will be evident below, will find a natural playground in the context of quantum simulations, preserving its analogue or digital character. If we iterate \( n \) times step 2 and step 3 with a suitable choice of gates and evolution times, we obtain the state \( \Phi = \frac{1}{\sqrt{2}}(|e\rangle \otimes U(t_{n-1}; t_0)|\phi\rangle + |g\rangle \otimes \tilde{U}_c^0|\phi\rangle) \), step 3 in Fig. 1. We show now how to apply this result to the case of non-Hermitian operators, independent of their unitary character, by considering the linear superpositions of Hermitian objects as in Eq. (4).

It is easy to see that, by using the composition property \( U(t_k; t_{k-1}) = U(t_{k-1}; 0)U(t_k; 0) \), Eq. (2) corresponds to a general construction relating \( n \)-time correlations of system operators \( \tilde{U}_c^k \) with two one-time ancilla measurements. In order to explore its depth, we shall examine several classes of systems and suggest concrete realizations of the proposed algorithm. The crucial point is establishing a connection that associates the \( \tilde{U}_c^k \) unitaries with \( \theta_k \) operators.

Starting with the discrete variable case, e.g. spin systems, and profiting from the fact that Pauli matrices are both Hermitian and unitary, it follows that

\[
\tilde{U}_c^n|\Omega_{\tau_m} = \pi/2\rangle = \exp\left(-\frac{i}{\hbar}H_m \tau_m\right)|\Omega_{\tau_m} = \pi/2\rangle = -i\theta_m, \tag{3}
\]

where \( H_m = \hbar \Omega \theta_m \), \( \Omega \) is a coupling constant, and \( \theta_m \) is a tensor product of Pauli matrices of the form \( \theta_m = \sigma_{m_1} \otimes \sigma_{m_2} \otimes \ldots \otimes \sigma_{m_n} \) with \( m_1, m_2, \ldots, m_n \in \{0, 1\} \), and \( \sigma_0 = I \). In consequence, the controlled quantum gates in step 2 correspond to \( U_c^n|\Omega_{\tau_m} = \pi/2\rangle = \exp\left(-\frac{i}{\hbar}|g\rangle\langle g| \otimes \Theta_0 \sigma_m \right) \), which can be implemented efficiently, up to local rotations, with two Mølmer-Sørensen gates [31–34]. In this way, we can write the second line of Eq. (2) as

\[
(-i)^n \langle e\rangle \langle \theta_{n-1}(t_{n-1}) \theta_{n-2}(t_{n-2})...\theta_0(0)|\phi\rangle, \tag{4}
\]

which amounts to the measured \( n \)-time correlation function of Hermitian and unitary operators \( \theta_i \). We can also apply these ideas to the case of non-Hermitian operators, independent of their unitary character, by considering the linear superpositions of Hermitian objects as in Eq. (4).

We show how to apply this result to the case of fermionic systems. In principle, the previous proposed steps would apply straightforwardly if we had access to the corresponding fermionic operations. In the case of quantum simulations, a similar result is obtained via the Jordan-Wigner mapping of fermionic operators to tensorial products of Pauli matrices, \( b_{p,q}^\dagger \rightarrow \Pi_{r=1}^\tau \sigma_r^{\sigma_{pr}} \sigma_r^{\sigma_{q}} \) [35]. Here, \( b_{p,q}^\dagger \) and \( b_{p,q} \) are creation and annihilation fermionic operators obeying anticommutation relations, \( \{b_{p,q}, b_{p,q}^\dagger\} = \delta_{p,q} \). For trapped ions, a quantum algorithm for the efficient implementation of fermionic models has been recently proposed [34, 36, 37]. Then, we code \( \langle b_{p,q}^\dagger(t)b_{p,q}(0)\rangle = \langle \Phi| (\sigma_{0}^{\sigma_{pr}} \otimes \sigma_{0}^{\sigma_{q}} \otimes \ldots \otimes \sigma_{n}^{\sigma_{pr}} \otimes \sigma_{n}^{\sigma_{q}})|\Phi\rangle \), where \( (\sigma_{0}^{\sigma_{pr}} \otimes \sigma_{0}^{\sigma_{q}} \otimes \ldots \otimes \sigma_{n}^{\sigma_{pr}} \otimes \sigma_{n}^{\sigma_{q}})|\Phi\rangle = e^{\pm \frac{i}{\hbar}H_{0} \tau \sigma_r^{\sigma_{pr}} \sigma_r^{\sigma_{q}} \otimes \ldots \otimes \sigma_r^{\sigma_{pr}} \sigma_r^{\sigma_{q}} \otimes \sigma_r^{\sigma_{pr}} \sigma_r^{\sigma_{q}}} \). Now, taking into account that \( \sigma_{+} = \frac{1}{2}(\sigma_{x} \pm i\sigma_{y}) \), the fermionic correlator \( \langle b_{p,q}^\dagger(t)b_{p,q}(0)\rangle \) can be written as the sum of four terms of
the kind appearing in Eq. (4). This result extends naturally to multimode correlations of fermionic systems.

The case of bosonic $n$-time correlators requires a variant in the proposed method, due to the nonunitary character of the associated bosonic operators. In this sense, to reproduce a linearization similar to that of Eq. (3), we can write

$$\partial_{t\alpha} U^m[t = 0] = \partial_{t\alpha} \exp \left( - \frac{i}{\hbar} H_m \right) |t = 0 = -i \theta_m, \tag{5}$$

with $H_m = \hbar \theta_m$. Consequently, it follows that

$$\partial_{t\alpha} \cdots \partial_{t\alpha} \text{Tr} \left( |g \rangle \langle g| \Phi \right) |t = 0 = \left( -i \right)^n \text{Tr} \left( \theta_{n-1} \cdots \theta_0 \langle g \rangle \right), \tag{6}$$

where the label $(\alpha, \cdots, \beta)$ corresponds to spin operators and $(j, \cdots, k)$ to spin-boson operators. The right hand side is a correlation of Hermitian operators, thus substantially extending our previous results. For example, $\theta_m$ would include spin-boson couplings as $\theta_m = \sigma_m \otimes \sigma_{jm} \cdots \sigma_{m(a + a')}$.

The way of generating the associated evolution operator $U_m = \exp (-iH \Omega_m \tau_m)$ has been shown in [34, 36, 38]. Note that, in general, dealing with discrete derivatives of experimental data is an involved task [39, 40]. However, recent experiments in trapped ions [14, 15, 41] have already succeeded in the extraction of precise information from data associated to first and second-order derivatives.

The presented method works as well when the system is prepared in a mixed-state $\rho_0$, e.g. a state in thermal equilibrium [20, 21]. Accordingly, for the case of spin correlations, we have

$$\text{Tr} \left( |g \rangle \langle g| \rho \right) = \left( -i \right)^n \text{Tr} \left( \theta_{n-1} \cdots \theta_0 \langle g \rangle \right), \tag{7}$$

with

$$\rho = \cdots U(t_2 - t_1) U(t_1 - t_0) U(t_0) \rho_0 (U(e^{i\Omega \tau_1} - 1)^\dagger \cdots U(e^{i\Omega \tau_0} - 1)^\dagger \cdots \right) \tag{8}$$

and $\rho_0 = \frac{1}{2} (|e \rangle \langle e| + |g \rangle \langle g|) \otimes \rho_0$. If bosonic variables are involved, the analogue to Eq. (6) reads

$$\partial_{t\alpha} \cdots \partial_{t\alpha} \text{Tr} \left( |g \rangle \langle g| \rho \right) |t = 0 = \left( -i \right)^n \text{Tr} \left( \theta_{n-1} \cdots \theta_0 \langle g \rangle \right), \tag{9}$$

We will exemplify the introduced formalism with the case of quantum computing of spin-spin correlations of the form

$$\langle \sigma_i^j (t) \sigma_i^j (0) \rangle, \tag{10}$$

where $k, l = x, y, z$, and $i, j = 1, \ldots, N$, $N$ being the number of spin-particles involved. In the context of spin lattices, where several quantum models can be simulated in different quantum platforms as trapped ions [11–13, 16, 42, 43], optical lattices [10, 44, 45], and circuit QED [46–49], correlations like (10) are a crucial element in the computation of, for example, the magnetic susceptibility [20–22]. In particular, with our protocol, we have access to the frequency-dependent susceptibility $\chi_\sigma \sigma$, that quantifies the linear response of a spin-system when it is driven by a monochromatic field. This situation is described by the Schrödinger equation $i\hbar \partial \psi = (H + f \sigma_i \sigma^j \alpha e^{i\omega t}) \psi$, where, for simplicity, we assume $H \neq H(t)$. With a perturbative approach, and following the Kubo relations [20, 21], one can calculate the first-order effect of the perturbation acting on the $j$-th spin in the polarization of the $i$-th spin as

$$\langle \sigma_i^j (t) \rangle = \langle \sigma_i^j (t) \rangle_0 + \chi_\sigma \sigma f \omega e^{i\omega t}. \tag{11}$$

Here, $\langle \sigma_i^j (t) \rangle_0$ corresponds to the value of the observable $\sigma_i^j$ in the absence of perturbation, and the frequency-dependent susceptibility $\chi_\sigma \sigma$ is

$$\chi_\sigma \sigma = \int_0^\infty ds \phi_{\sigma, \sigma} (t - s) e^{i\omega (s - t)} \tag{12}$$

where $\phi_{\sigma, \sigma} (t - s)$ is called the response function, which can be written in terms of two-time correlation functions,

$$\phi_{\sigma, \sigma} (t - s) = \frac{1}{\hbar} \text{Tr} \left( \langle \sigma_i^j (t) \sigma_i^j (0) \rangle \right), \tag{13}$$

with $\rho = U(t) \rho_0 U(t)^\dagger$, $\rho_0$ being the initial state of the system and $U(t)$ the perturbation-free time-evolution operator [20]. Note that for thermal states or energy eigenstates, we have $\rho = \rho_0$. According to our proposed method, and assuming for the sake of simplicity $\rho = \Phi$, the measurement of the commutator in Eq. (13), corresponding to the imaginary part of $\langle \sigma_i^j (t) \sigma_i^j (0) \rangle$, would require the following sequence of interactions: $|\Phi \rangle \rightarrow U_c U_c U(t - s) U_c |\Phi \rangle$, where $U_c = e^{-i(\Omega \tau_1)} |\sigma_i \Omega \rangle$, $U(t) = e^{-iHt}$, and $U_c = e^{-i(\Omega \tau_2)} |\sigma_i \Omega \rangle$, for $\Omega \tau = \pi/2$. After such a gate sequence, the expected value in Eq. (13) corresponds to $-1/2 \langle \Phi | \sigma_i | \Phi \rangle$. In the same way, second-order corrections to the linear response of Eq. (11) can be calculated through the computation of three-time correlation functions of the form $\langle \sigma_i^j (t_2) \sigma_i^j (t_1) \sigma_i^j (0) \rangle$. In this case, one should perform the evolution $|\Phi \rangle \rightarrow U_c U_c U(t_2 - t_1) U(t_1) U_c |\Phi \rangle$, where $U_c = e^{-i(\Omega \tau_2)} |\sigma_i \Omega \rangle$, $U(t) = e^{-iHt}$, and $U_c = e^{-i(\Omega \tau_1)} |\sigma_i \Omega \rangle$ for $\Omega \tau = \pi/2$. The searched time correlation now corresponds to the quantity $1/2 \langle i \Phi \sigma_i \Phi | \Phi - \Phi \sigma_i \Phi \rangle$.

The same techniques can be used to study the effect of external perturbations onto the motional degrees of freedom of the involved particles. For example, the time correlation $\langle (a_i^+ + a_i^\dagger) (t - s) \sigma_i \rangle$, where $(a_i + a_i^\dagger) (t - s) = e^{iH(t - s)} (a_i + a_i^\dagger) e^{-iH(t - s)}$, will enter in the magnetic susceptibility $\chi_{a \sigma a \sigma} \sigma$ through the response function $\phi_{\sigma, a \sigma, a \sigma} (t - s)$. The latter can be written as in Eq. (13) but replacing the operator $\sigma_i^j (t - s)$ by $(a_i + a_i^\dagger) (t - s)$. The linear response of the system is now

$$\langle (a_i + a_i^\dagger) \rangle |_0 + \chi_{a \sigma a \sigma} \sigma f \omega e^{i\omega t}. \tag{14}$$
In this case, the gate sequence for the measurement of the associated correlation function \( \langle \sigma_i \sigma_j \rangle \) reads

\[
\Phi \rightarrow U_c \Phi \rightarrow U(t-s)U_c^\dagger \Phi,
\]

where \( U_c = e^{-\frac{i}{\hbar}\int \Omega(t) dt} \), \( U(t-s) = e^{-\frac{i}{\hbar} \int \omega(t) dt} \), and \( U_c^\dagger = e^{-\frac{i}{\hbar} \int \omega_c(t) dt} \). The time correlation is now obtained through the first derivative \(-1/2\partial \Omega_{ij}(\Phi \sigma_i \sigma_j + i\dot{\langle \Phi | \sigma_i \sigma_j \rangle})\). Equations (11) and (14) can be extended to describe the effect on the system of light pulses containing frequencies in a certain interval \((\omega_0, \omega_0 + \delta)\). Here, Eqs. (11) and (14) correspond to

\[
\langle \sigma_i^k(t) \rangle = \langle \sigma_i^k(0) \rangle + \int_{\omega_0}^{\omega_0+\delta} \chi_{\sigma_i^k} \tilde{\chi}_{\sigma_j^\sigma} f_\omega e^{i\omega t} d\omega,
\]

and

\[
\langle \sigma_i^k(t-s) \rangle = \langle \sigma_i^k(0) \rangle + \int_{\omega_0}^{\omega_0+\delta} \chi_{\sigma_i^k} \tilde{\chi}_{\sigma_j^\sigma} f_\omega e^{i\omega t} d\omega.
\]

Note that despite the presence of many frequency components of the light field in the integrals of Eqs. (15, 16), the computation of the susceptibilities, \( \chi_{\sigma_i^k} \tilde{\chi}_{\sigma_j^\sigma} \), just requires the knowledge of the time correlation functions \( \langle \sigma_i^k(t) \sigma_j^\dagger(0) \rangle \) and \( \langle \sigma_i^k(t-s) \rangle \), which can be efficiently calculated with the protocol described in Fig 1. In this manner, we provide an efficient quantum algorithm to characterize the response of different quantum systems to external perturbations. Our method may be related to the quantum computation of transition probabilities \( \langle \sigma_i(t) \rangle = \langle \sigma_i^k(t) \rangle \langle \sigma_j^\dagger(t) \rangle = \langle \sigma_i^k(t) \rangle \langle \sigma_j^\dagger(t) \rangle 
\]

between initial and final states, \( |i\rangle \) and \( |f\rangle \), with \( P(t) = U(t) \dagger |f\rangle \langle i| U(t) \), and to transition or decay rates \( \dot{\langle \sigma_i^k(t) \rangle} \), the J. J. Sakurai, Modern Quantum Mechanics (Addison-Wesley Publishing Company, 1994).
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