

Time evolution and use of multiple times in the N -body problem

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Under certain conditions it is possible to describe time evolution using different times for different particles. Use of multiple times is optional in the independent particle approximation, where interparticle interactions are removed, and the N -particle evolution operator factors into N single-particle evolution operators. In this limit one may use either a single time, with a single energy-time Fourier transform, or N different times with a different energy-time transform for each particle. The use of different times for different particles is fully justified when coherence between single-particle amplitudes is lost, e.g., if relatively strong randomly fluctuating residual fields influence each particle independently. However, when spatial correlation is present the use of multiple times is not feasible, even when the evolution of the particles is uncorrelated in time. Some calculations in simple atomic systems with and without spatial and temporal correlation between different electrons are included.

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I. INTRODUCTION

A single time is, in principle, appropriate for all particles in any N -body system, no matter how complex the system. In practice, however, large systems are often approximately treated as a collection of uncorrelated or weakly connected subsystems. In such cases it is easier, and often sensible, to use N independent times for the independent subsystems, rather than to use a single time. In this paper we discuss conditions under which it is appropriate to use multiple times in the quantum N -body problem.

The basic condition required for use of N different times is that the N particles do not interact with one another. This limit is called the independent particle approximation (IPA) [1–13]. This spatially uncorrelated independent particle limit differs from the independent time approximation (ITA) [14,15], in which the time evolution of different particles is decoupled. Here we differentiate between spatial and temporal correlation in quantum many-body systems and their effect on the use of different times for different particles.

In many applications of conventional scattering theory, the energy domain is used [16,17]. However, it is sensible to also study dynamic quantum systems in the conjugate time domain, namely, to address how quantum particles are interconnected in time. In particular, problems that involve time correlation are more naturally suited to the time domain. Generally, such problems arise in applications ranging from sequential transitions in molecules [18], to formation and decay of coherent N -body states [19], and to quantum computing [20].

In this paper we briefly review the basic formulation of correlation in space and time. The use of different times for different particles is connected to the notion of interparticle

correlations. Examples are discussed where the use of multiple times is optional, where use of multiple times is fully justified, and finally where such use is not appropriate. We also present some calculations with and without spatial and temporal correlation.

II. THEORY

A. Formulation

Consider a system of N particles coupled to an external environment via some $V(t)$. Examples include N interacting particles in the presence of an external field, or a correlated N -electron atomic target interacting with an incident photon or a charged particle. The Hamiltonian for such a system is

$$H = H_0 + V(t),$$

$$H_0 = \sum_j^N \left(H_{0j} + \sum_{k>j} v_{kj} \right). \quad (1)$$

Here the N particles are interconnected by mutual two-body interactions, v_{ij} , which provide spatial correlation between the particles. In an atomic target, for example, $v_{ij} = 1/r_{ij}$ is an electron-electron Coulomb interaction. We generally assume that $V(t)$ may be written as $V(t) = \sum_j^N V_j(t)$. In the independent particle limit the $V_j(t)$ reduce to one-particle operators which commute with one another [13].

The time-dependent wave function for this N -body system is given by

$$\Psi(t) = U(t, t_0) \Psi(t_0), \quad (2)$$

where the time dependence is carried by the evolution operator [16,17]

$$U(t, t_0) = T e^{-i \int_{t_0}^t V(t) dt}$$

$$= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^t dt_n \cdots \int_{t_0}^{t_n} dt_1 T V(t_n) \cdots V(t_1). \quad (3)$$

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All time dependence of the system is carried by $TV(t_n)\cdots V(t_1)$. Here T is the Dyson time ordering operator [17,21,22], which provides a constraint that connects the $V(t)$ in a pairwise fashion to enforce causality. Specifically, $TV(t_2)V(t_1) = V(t_2)V(t_1)$ for $t_2 - t_1 > 0$, $TV(t_2)V(t_1) = 0$ for $t_2 - t_1 < 0$, and $U(t_2, t_1) = 0$ for $t_2 - t_1 < 0$. Time ordering interconnects the time evolution of different particles [14] and thus provides correlation in time between different particles.

In the independent particle approximation (IPA), the v_{kj} interparticle interactions in Eq. (1) go to zero. Then the total Hamiltonian reduces to a sum of single-particle operators and, using separation of variables, the total wave function may be factored into a single product of single-particle terms [13],

$$\Psi \rightarrow \prod_j^N \Psi_j(t). \quad (4)$$

This independent particle approximation [1–13] has been used for over 30 years and is well established.

The ITA is more recent [14,15]. In Eq. (3) if there is no time ordering between different particles, e.g., $T \rightarrow T_{av} = 1$, then the interactions, $V_j(t)$, for different particles all commute and may be put in any order, so that interactions for each particle may be grouped together. Applying this limit, with $T \rightarrow T_{av} = 1$ only between different electrons,

$$\begin{aligned} \lim_{T \rightarrow T_{av}} U(t, t_0) &= \lim_{T \rightarrow T_{av}} T e^{-i \int_{t_0}^t \sum_j^N v_j(t) dt} \\ &= \prod_j^N \left(T e^{-i \int_{t_0}^t v_j(t) dt} \right) = \prod_j^N U_j(t, t_0). \end{aligned} \quad (5)$$

This defines the independent time approximation, where particles evolve independently in time. In this case time ordering is retained only in single-particle time evolution. As explained below, this independent time approximation does not necessarily require use of different times for different particles.

B. Examples of multiple times

In this section we give some examples concerning the use of multiple times. In the first example we consider the case of the independent particle approximation where multiple times may be used, but where such use is optional. In the independent time approximation the use of multiple times is restricted by the initial asymptotic wave function. Mandatory use of multiple times is illustrated in the third case where random fields irretrievably decouple time-dependent amplitudes for different particles. In our last example we show how a single time is recovered by turning on interparticle interactions, i.e., correlation.

1. Equivalence of single and multiple times for spatially uncorrelated particles

As a first example we consider the simplest case of IPA [12,23–28]. In the uncorrelated, independent particle approximation there are no interactions between the particles in the system. This corresponds to $v_{kj} \rightarrow 0$ or $v_{kj} \ll V_j(t)$ in Eq. (1), so that

$$\begin{aligned} H_0 &\rightarrow \sum_j^N H_{0j}, \\ H &\rightarrow \sum_j^N [H_{0j} + V_j(t)] = \sum_j^N H_j(t). \end{aligned} \quad (6)$$

Since the H_j terms now commute with one another at all times [including t_0 where $V(t_0)$ is usually zero],

$$\begin{aligned} \Psi(t) &= U(t, t_0) \Psi(t_0) \rightarrow \prod_j^N \Psi_j(t) = \prod_j^N U_j(t, t_0) \Psi_j(t_0), \\ U(t, t_0) &\rightarrow \prod_j^N U_j(t, t_0). \end{aligned} \quad (7)$$

Here the uncorrelated particles evolve independently. Since $\Psi(t)$ is separable, each $\Psi_j(t)$ may be evaluated using a different time t_j corresponding to

$$\Psi(t) = \prod_j^N \Psi_j(t) \rightarrow \prod_j^N \Psi_j(t_j). \quad (8)$$

In each of the ψ_j the time t may be changed without influencing any of the other ψ_j . Thus, in the independent particle limit the use of different times for different particles is allowed, but not required.

We note that each individual $\Psi_j(t)$ may be changed by an arbitrary overall phase, $\delta_j(t)$, which nevertheless leaves just one overall phase, $\delta(t) = \sum_j \delta_j(t)$, in the total wave function $\Psi(t)$. In the trivial case of product of plane waves, for example, the $\Psi_j(t) = e^{iE_j(t-t_0)}$ may each be modified by random phase $e^{i\delta_j(t)} = e^{iE_j t_j}$ with a random t_j . The basic idea is that whenever an amplitude is expressed as a simple product of single-particle terms there is no phase coherence between the individual terms in this product.

In the independent particle limit one may generally use either a single Fourier transform, $\int e^{iEt} f(t) dt$, or N independent Fourier transforms, $\int e^{iE_j t_j} f(t_j) dt_j$, where $f(t)$ is an arbitrary function. The single transform uses a single time, while the N independent transforms use N different times, one for each of the N particles.

2. Time and independent time evolution

In ITA, spatial correlation may be present so that

$$U(t, t_0) \rightarrow \prod_j^N U_j(t, t_0), \quad (9)$$

but $\Psi(t_0) - \prod_j^N \Psi_j(t_0)$ may or may not be zero. If $\Psi(t_0) = \prod_j^N \Psi_j(t_0)$, then one recovers the independent particle approximation discussed above and independent times may be used. If $\Psi(t_0) \neq \prod_j^N \Psi_j(t_0)$, then the phases between the individual particles do not simply lead to a single overall phase and independent times may not be used. If the times of the particles are correlated at t_0 , they remain correlated in the independent time approximation. In other words, when Eq. (9) holds, any time correlation rests with the asymptotic wave functions and not with the time evolution itself. While the time evolution of particle amplitudes is decoupled in the independent time approximation, whether particles can be characterized by one time or by multiple times depends entirely on the asymptotic conditions. Independent time evolution of different particles does *not* mean that the particles may be described by different times.

3. Transition from one time to multiple times

In this subsection we consider conditions that fully justify the use of different times for different particles. This is done by introducing randomly fluctuating fields that independently vary the phase for different, separated, uncorrelated particles. Here these random fields are stronger than either the interparticle interactions, v_{ij} , or the external interactions, $V_j(t)$. An example is removal and separation of electrons from an atom into regions with independent, randomly fluctuating, relatively strong electromagnetic fields.

Let us consider N correlated particles, initially coherent, interacting with an initially strong field, $V(t)$, that is damped at large values of t . By coherent we mean that the phase differences for each of the particles are well defined and, if they change in time, they change in a clearly prescribed way. For coherent particles only a single time parameter is needed. Consider an interaction $V(t)$ that goes to zero at times large compared to an interaction time t_V . This t_V could, for example, be the duration of a collision of an atom with an incoming projectile. Since the N particles are initially coherent, Ψ is described by a single time at t_0 , namely, $\Psi(t_0)$. Then for all $t > t_V > t_0$,

$$\Psi(t) = U(t, t_0) \Psi(t_0) \tag{10}$$

is described by the evolution in a single time parameter. In such a system the particles might be separated by large distances and thus become decoupled. Then the independent time approximation holds, and $U(t, t_V) \rightarrow \prod_j^N U_j(t, t_V)$.

Now, for the separated particles the interaction $V(t)$ goes to zero for $\tau \gg t_V$. Then fluctuating residual fields, e.g., random stray fields, $\mathcal{V} = \sum_j \mathcal{V}_j$ [not specified in Eq. (1)] will be larger than $V(\tau)$. The only required feature of the \mathcal{V}_j is that the action integrals $\int_\tau \mathcal{V}_j dt$ are independently random. After a sufficiently long time t_{random} defined by $\int_\tau^{\tau+t_{random}} \mathcal{V} dt \gg 1$, the action of these random fields cannot be neglected. Mathematically this corresponds to

$$U(\tau, t_V) = \prod_j^N \left(T e^{-i \int_{t_V}^\tau \mathcal{V}_j dt} \right)_j = \prod_j^N e^{i \delta_j(\tau, t_V)}, \tag{11}$$

where the δ_j are random. Since the \mathcal{V}_j are independently random, the phases will evolve randomly for each particle. Time correlation between different particles is now irreversibly lost, since the phase terms are now random. Different particles must be described by different times.

The time it takes for this decoherence in time to take effect can be estimated by

$$t_{decoh} = \int_{-\infty}^{\infty} \gamma(t') dt', \tag{12}$$

where $\gamma(t')$ is a normalized cross correlation function [29] for the time evolution given by

$$\gamma(t') = \frac{\langle U_j(t+t', t_0) U_k(t, t_0) \rangle}{\langle U_j(t, t_0) U_k(t, t_0) \rangle}, \tag{13}$$

where $\langle \dots \rangle$ denotes an average over t' . Of all possible jk terms, the γ function that falls off most slowly in time is used in Eq. (12). After a time large compared to t_{decoh} , coherence between the various particles is lost via the influence of randomly fluctuating fields for each particle, and it is sensible to use different times for different particles.

4. Transition from N incoherent times to one coherent time

In the previous examples we have illustrated cases where multiple times may be used in the dynamic N -body problem. Here we consider a case where multiple times may not be used.

Consider a system of N independent particles described initially by $\Psi(t_0) = \prod_j \Psi_j(t_{j0})$. The various Ψ_j 's are initially incoherent, as denoted here by different t_{j0} . Let the correlation between these particles via interactions, $v_{ij}(\vec{r}_{ij}, t)$, turn on over some interval of time. This could be done, for example, by using a positively charged nucleus to attract N separated electrons to form a neutral atom.

Since v_{ij} is now nonzero, $U(t, t_0)$ is no longer a product of one-particle evolution operators. The corresponding $V_j(t_j)$ no longer commute [13,30] for different j . This is especially clear in the interaction representation where

$$V_j(t) = e^{-iH_0 t} V_j(t_0) e^{iH_0 t}, \tag{14}$$

where $V_j(t)$ is a simple scalar function, such as a Coulomb interaction $Z/|\vec{R}(t) - \vec{r}_j|$ between a projectile at \vec{R} and an electron at \vec{r}_j . In contrast, $V_j(t)$ is a many-body operator due [13] to the presence of v_{ij} in H_0 . Since H_0 includes v_{ij} , H_0 does not commute with $V_j(t)$, and $V_j(t)$ does not commute with $V_k(t)$. As a consequence

$$e^{-i \int_{t_0}^t \sum_j^N V_j(t) dt} \neq \prod_j^N e^{-i \int_{t_0}^t V_j(t) dt}. \tag{15}$$

The evolution operator for the system cannot be written in product form, i.e.,

$$U(t, t_0) \neq \prod_j^N U_j(t, t_0). \tag{16}$$

Now the time evolution of the various particles is coupled. The Dyson time ordering operator T may not be replaced by its average value T_{av} . This causes time correlation to develop between the U_j 's. If $U(t, t_0)$ cannot be written as a single product, the relative phases between the various terms become significant. Now $\Psi(t) \neq \prod_j^N \Psi_j(t_j)$. The various t_j are coupled. A single time t is now required.

The time required for such time correlation to develop may be estimated by a time t_{cor} ,

$$t_{cor} = \int_{-\infty}^{\infty} \gamma(t') dt', \quad (17)$$

where γ is the largest normalized cross correlation function defined by Eq. (13) with $v_{ij}(t)$ present in $U(t, t_0)$. After a time large compared to t_{cor} , coherence is established between the various particles and the use of different times for different particles is no longer feasible. A single time is now both necessary and sufficient. For example, for $t > t_{cor}$ all separated electrons may be settled into the ground state of an atom.

III. CALCULATIONS

In this section we present calculations that illustrate the effect of correlation in space and correlation in time for a relatively simple few-body system, namely the two-electron case with atomic helium. We expect the main points to hold for any system of N bodies. The helium atom we consider interacts with a moderately fast incoming proton. We present calculations in three stages: independent particle approximation, then independent time approximation, and finally full calculations. In our first case correlation is fairly weak, in the next case spatial correlation is strong but time correlation is small, and finally both temporal and spatial correlation are strong.

A second-order calculation is accurate if the incident protons are moderately fast. In this case the second-order scattering amplitude for any transition from an initial state $|i\rangle$ to any final state $|f\rangle$ is given by

$$f_2 = \langle f | V + V \frac{1}{E - E_0 + i\eta} V | i \rangle. \quad (18)$$

Time correlation is carried [30] by the quantum energy fluctuation, corresponding to the principal-value contribution of $1/(E - E_0 + i\eta) = i\pi\delta(E - E_0) - \mathcal{P}_v/(E - E_0)$. The Fourier transform of energy fluctuation $\mathcal{P}_v/(E - E_0)$ term is the operator $\Delta T = T - T_{av}$. It is this part of the time ordering operator that entangles the time evolution of the two electrons. We do not expect these particular effects of time correlation to be present in classical calculations [8,9], since the principal-value term corresponds to off-shell quantum fluctuations in the energy due to short-lived transitions in intermediate states that are not present in classical calculations.

In the calculations presented in this paper the electron exchange due to the indistinguishability of electrons is fully included by antisymmetrizing the electronic wave functions. Conceptually, however, it is convenient to ignore such ex-

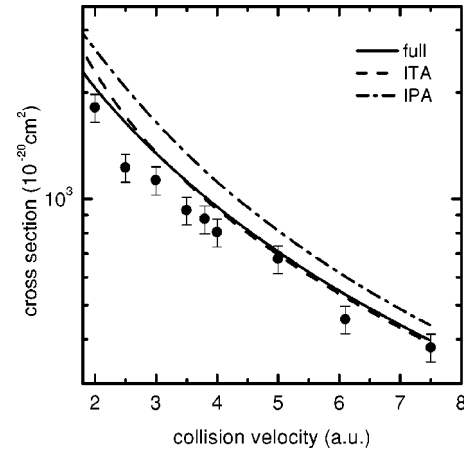


FIG. 1. Cross sections for $1s$ - $2p$ excitation of a single electron in helium by proton impact as a function of the velocity of the incoming proton. IPA denotes the independent particle approximation and ITA denotes the independent time approximation. Experimental data are from the group of Bruch *et al.* [23].

change effects as we have done above. This simplifies the meaning of “an electron” and “an electron transition” and allows one to regard electrons as distinguishable. Inclusion of exchange is straightforward, but adds complexity both conceptually and mathematically. In high-energy atomic collisions the effects of exchange are often small.

The first case we consider is the cross section for excitation of one electron in helium by a moderately fast incoming proton shown in Fig. 1. The full second Born calculation falls 15% or so below the independent particle approximation and is quite close to the independent time approximation, except at the lowest velocities, where the second Born approximation is expected to break down. As explained above different times may be used for different electrons when the independent particle approximation is valid. The use of different times for the two electrons is fairly accurate for case shown in Fig. 1. While the effect of time correlation between particles is present in single-particle transitions, it is our experience that the effect is more obvious and easier to detail in cases with multi-electron transitions.

The case we consider next is double excitation of helium by proton impact shown in Fig. 2. Here the independent particle approximation is not uniformly accurate. In the independent time approximation, time correlation is removed by dropping principal-value contributions defined below Eq. (18). Spatial correlation is retained in the independent time approximation. Both of these approximations are compared to a full second Born calculation exact through second order in $V(t)$ and including all orders in the correlation interaction v_{ij} . This calculation is described in detail elsewhere [31]. The difference between the full calculation and the independent time approximation is quite small in this case. However, even though the electrons evolve independently in time, they may not be characterized by different times, as explained in Sec. II B 2 above.

In the last case we present in Fig. 3 calculations for ionization occurring together with excitation of a second electron to the $n=4$ excited $4p$ level in He^+ . In this case the projec-

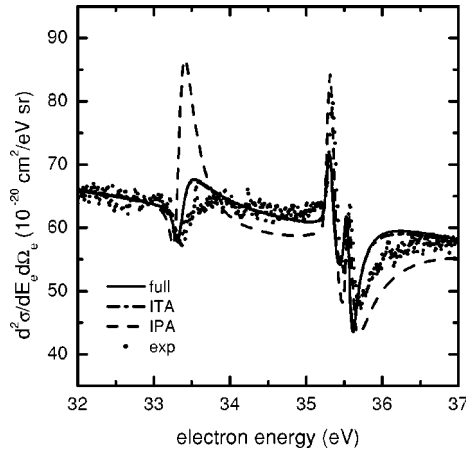


FIG. 2. Cross sections for autoionizing $2s^2(^1S)$, $2p^2(^1D)$, and $2s2p(^1P)$ resonances of helium in the electron emission spectrum excited by 100 keV proton impact. The electron angle of emission is 17° and the cross section shown is averaged over all projectile scattering angles. Experimental data are from the group of Bordenave-Montesquieu *et al.* [31].

tile is a fast proton. Again we see that the independent particle approximation, where spatial electron-electron correlation is removed, is not very accurate for this two electron transition. In this case the independent time approximation is also not especially accurate. Consequently there is a significant correlation in the time evolution of the two electrons, so that time correlation is not weak and the use of a single time is needed. New data for this cross section may be available soon [32].

In many cases in fast collisions spatial correlation is more important than time correlation [14,15,30,33,34]. At somewhat lower energies the role of temporal correlation is expected to be generally stronger, although higher-order terms in the expansion in $V(t)$ may also be significant. We emphasize that use of the independent time approximation provides computational and conceptual simplification. In particular, calculations using the independent time approximation [14] require less computational time than calculations including

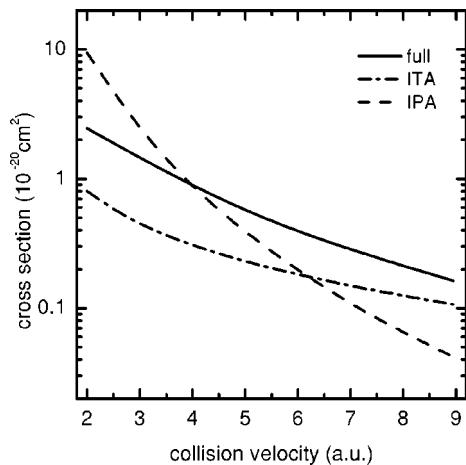


FIG. 3. Cross section for ionization together with excitation to the $n=4p$ level of He^+ by impact of fast protons.

time correlation. In the case of the relatively simple calculations presented here, the difference is over two orders of magnitude. For more complex systems the difference is expected to be greater [35].

IV. DISCUSSION AND SUMMARY

For scattering by an external $V(t)$, it has been argued that time t enters in a purely classical way [36]. While we agree with the mathematical details of this argument [37], we point out that the energy propagator, $1/E-H+i\eta$ couples the quantum system to an asymptotic environment via the principal-value contribution from $i\eta$. This term determines the direction of time, i.e., whether there are outgoing or incoming scattering waves. It is straightforward to show [14] that the Fourier transform of the principal-value contribution produces time correlation. This is a quantum effect corresponding to energy nonconservation, which is allowed for short times in intermediate states. This effect requires interparticle correlation [30]. The effect is observable [33].

Unlike classical physics, in quantum systems one may not characterize time as an observable interval between localized events. Pauli's well-known observation about the impossibility of defining a self adjoint operator for time in any system with a bound spectrum has led to a discussion of operators for different time parameters [38], including arrival and passage times. While time is not always physically observable in quantum systems, it can be useful [39] to identify a variety of different time parameters, which may be delocalized in quantum systems. These include a correlation time t_{cor} a time required to develop time correlation between particles; a random time t_{random} a time required for random fields to dominate over decaying interactions, $V(t)$; an interaction time t_V , the duration of the interaction $V(t)$; and a decoherence time t_{decoh} , a time sufficient for phase decoherence between uncorrelated particles to take effect. Other time parameters can enter as well, such as the orbital period of a bound particle, decay times for excited states, recovery times for detectors, coherence and bunching times of beams, and various macroscopic times for various stages of an experiment.

In this paper we have seen interplay between random phase incoherence and independent times. We note that the concepts of correlated and non-random are similar. In particular both have the same mathematical definition. Correlated and nonrandom both mean that for some observable property P such as the probability of a transition $P(1,2,\dots,N) \neq \prod_j P_j(j)$. Entanglement is also defined in the same manner.

In summary, we have shown that in the absence of spatial correlation between particles, multiple particles may be described by either a single time or by multiple times. If time ordering between different particles is removed, then the time evolution operators may be expressed as a product of single-particle time evolution operators and the particles evolve independently in time. However, independent time evolution of different particles does not mean that the particles may be described by different times. Specifically, different times may not be used for different particles in the

absence of time correlation when the initial asymptotic state of the system is spatially correlated. Thus there is an asymmetry in spatial and temporal correlation: time correlation between particles is forbidden in the absence of spatial correlation, but spatial correlation between particles is permitted in the absence of time correlation. Calculations illustrating the effects of spatial and temporal correlation have been presented. When relatively strong random fields independently change the phase of the wave function for each particle the use of multiple times is fully justified. When spatial correla-

tion is strong, the time evolution of different particles is correlated. Then a single time is needed.

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