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# Evolution of a Quantum System: Lifetime of a Determinant*

Peter C. Lichtner†
*Institut für Kernphysik der Universität Mainz, Mainz, West Germany*

and

James J. Griffin‡
*Universität Giessen, Giessen, West Germany, and The Hahn-Meitner-Institut, Berlin, West Germany, and University of Maryland, College Park, Maryland 20742*

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A measure of the "dependency" of a many-particle system is defined and its time dependence is evaluated for systems initially described by a single Slater determinant. An uncertainty product between the energy spread of the initial determinant and the lifetime of a system's independence is established. Numerical estimates of some lifetimes are given. They are not so long as to be reassuring for nuclear time-dependent Hartree-Fock calculations. Each separate case ought to be checked.

In the analysis of nucleon heavy-ion processes by means of time-dependent Hartree-Fock (TDHF) numerical models,[1,2] the wave function of the system is assumed initially to be well described by a single determinant, and is evolved subsequently in time under the specific assumption that the wave function remains a determinant. On the other hand, even assuming that the description of the system wave function initially (i.e., at $t = t_0$) as a single Slater determinant $\psi_0$ were exact,[3] the system in fact evolves forward in time, not as dictated by the Hartree-Fock approximate Hamiltonian, $\mathcal{H}^{\mathrm{HF}}$, but according to the true, exact Hamiltonian of the system, $H^{\mathrm{EX}}$.

Structurally these two Hamiltonians differ in that the Hartree-Fock Hamiltonian involves only single-nucleon potentials (obtained, at the expense of the linearity of the Hamiltonian, by averaging over the wave functions of the nucleons in the system), whereas the true Hamiltonian is generally assumed to involve two-nucleon interactions. This difference in structure guarantees a very specific difference in the time evolutions of the two descriptions: The true evolution will, as time progresses, introduce into the wave function particle-particle correlations not describable within a single determinant, whereas the approximate Hartree-Fock one-particle Hamiltonian, by construction, generates at each instant a new single determinant from the old one.

A many-particle wave function, $\psi(t)$, can be written as a single determinant, if and only if the matrix

$$\mathfrak{D}_{\alpha\beta} = (\rho - \rho^2)_{\alpha\beta} = [\rho_{\alpha\beta} - \textstyle\sum_\lambda \rho_{\alpha\lambda}\rho_{\lambda\beta}] \qquad (1)$$

is identically zero, where $\rho_{\alpha\beta}(t)$ is the single-particle density matrix defined by

$$\rho_{\alpha\beta}(t) = \langle \psi(t) | a_\beta{}^\dagger a_\alpha | \psi(t) \rangle . \qquad (2)$$

We define the "dependency," per particle, of any wave function by the number[4]

$$D = A^{-1}\mathrm{Tr}\mathfrak{D} = A^{-1}\textstyle\sum \hat{\mathfrak{D}}_{\alpha\alpha}. \qquad (3)$$

By virtue of the Hermiticity of $\rho$ (which allows $\rho$ to be diagonalized into a real matrix) and the Fermi statistics of the problem (which guarantees that every diagonal element of $\rho$ lies in the range $0 \leq \rho_{\alpha\alpha} \leq 1$, and therefore that every diag-

onal element, $D_{\alpha\alpha}$, is non-negative), the number $D$ can vanish only when the operator $\hat{\mathfrak{D}}$ vanishes. Thus zero dependency, $D=0$, also implies that the wave function can be expressed as a single Slater determinant. A finite nonzero value of the dependency, $D$, on the other hand, guarantees that the wave function cannot be expressed as a single determinant.

Thus the finite value of $D$ for the exact solution will deviate in time from the zero value which characterizes the approximate, single-determinant, Hartree-Fock solution. Its time dependence therefore allows a natural measure of the time over which one can expect the TDHF approximation to provide a good approximation to the exact dynamical evolution.

To estimate the time over which the Hartree-Fock evolution may reasonably be expected to apply, we study the growth in time of the dependency, $D(t-t_0)$, in (3) as given by the Taylor expansion:

$$D(t-t_0)=D(t_0)+(t-t_0)D^{(1)}(t_0)+(2!)^{-1}(t-t_0)^2D^{(2)}(t_0)+\dots. \tag{4}$$

By hypothesis $D(t_0)=0$: $\psi(t_0)$ is assumed to be a determinant. In addition, one finds by direct calculation that

$$D^{(1)}(t_0)=0, \tag{5}$$

whenever $\psi(t_0)$ can be written as a single determinant $[D(t_0)=0]$. This result follows from the evaluation of

$$D^{(n)}(t_0)=-\left[\frac{d^n}{dt^n}\{\textstyle\sum_{\alpha\beta}|\langle\psi(t)|a_\beta^\dagger a_\alpha|\psi(t)\rangle|^2\}\right]_{t=t_0}, \tag{6}$$

for $n=1$, by means of

$$d\psi(t)/dt=-iH^{EX}d(t), \tag{7}$$

and evaluation of commutators of the form $[H^{EX}, a_\beta^\dagger a_\alpha]$. Thus the early-time behavior of $D$ is given by

$$D(t-t_0)=\tfrac{1}{2}(t-t_0)^2D^{(2)}(t_0)+\dots \tag{8a}$$

$$=[(t-t_0)/\tau_D]^2. \tag{8b}$$

The quantity $\tau_D$ defined here measures the "dependency lifetime" during which a substantial deviation from a pure independent-particle determinant grows into the wave function. It is calculated by means of (6) for $n=2$ and double commutators of the Hamiltonian with $a_\beta^\dagger a_\alpha$. One finds thereby that

$$\tau_D=\frac{\hbar}{2}\left\{\frac{1}{A}\sum_{\substack{(\mu<\nu)\in F\\(\sigma<\tau)\notin F}}|\bar{v}_{\mu\nu,\sigma\tau}|^2\right\}^{-1/2}, \tag{9}$$

where the set $F$ is the set of single-particle states filled in the determinant $\psi(t_0)$, and $\bar{v}_{\mu\nu,\sigma\tau}$ is the difference between the direct and exchange matrix elements of the two-nucleon interaction of the exact Hamiltonian.

An energy eigenstate of the true Hamiltonian is, of course, stationary in time. Indeed, a measure of the time for the growth of the dependency, $D$, of a wave function, such as $\tau_D$ in Eq. (9), might reasonably be expected, by virtue of the general complementarity of energy uncertainty and lifetime, to be closely related to the energy spread of the system described by $\psi(t_0)$. To see that this is indeed the case we have computed the energy spread (per particle),[4] as follows:

$$(\Delta E_0)^2=\frac{1}{A}\langle\psi(t_0)|H^2|\psi(t_0)\rangle-\frac{1}{A}\langle\psi(t_0)|H|\psi(t_0)\rangle^2, \tag{10}$$

$$=\frac{1}{A}\sum_{\substack{(\mu<\nu)\in F\\(\sigma<\tau)\notin F}}|\bar{v}_{\mu\nu,\sigma\tau}|^2+\frac{1}{A}\sum_{\substack{\mu\in F\\\sigma\notin F}}|\mathcal{H}_{\mu\sigma}{}^{HF}|^2. \tag{11}$$

The second term in Eq. (11) is positive semidefinite, and vanishes only when $\psi(t_0)$ is an eigenfunction of $\mathcal{H}(t_0)$. (This might occur for stationary-state or freely translating Hartree-Fock solutions, but not for nontrivial TDHF solutions, except perhaps at some specific point in time.) Thus from (11) and (9), one can write the complementarity product,

$$\Delta E_0\tau_D\geq\hbar/2, \tag{12}$$

relating the energy spread of the initial determinant with its lifetime for decay into nondeterminantal forms. We emphasize that the initial time $t_0$ may be arbitrarily chosen at any point along the path of a TDHF evolving determinant.

Precise estimation of $\tau_D$ by means of Eq. (9), or Eqs. (10) and (12), even for the simplest case of a single isolated nucleus, requires calculation of the stationary-state Hartree-Fock solutions for the Hamiltonian in question. Fortunately, some published Hartree-Fock calculations of nuclear ground states[5] report values for the quantity (10) and so allow immediate inference of the quantity $\tau_D$. Table I summarizes some examples of this kind.

TABLE I. Values of $(\Delta E_0)^2$, Eq. (10), from Ref. 5, and the corresponding estimated dependency times, $\tau_D$, from Eqs. (9) and (12) for isolated single nuclei of the type noted. Since these times are probable upper bounds on $\tau_D$ values which are expected to apply to nuclei to collision (see text), and since they are comparable to (and surely not much greater than) the times for nuclear heavy-ion collisions, they support a cautious view of TDHF numerical models for such collisions.

| Nucleus | $(\Delta E_0)^2$ (MeV$^2$) | $\tau_D=\hbar/2(\Delta E_0)$ ($10^{-22}$ sec) |
|---|---|---|
| $^{20}$Ne | 0.54 | 4.4 |
| $^{24}$Mg | 0.71 | 3.9 |
| $^{28}$Si | 0.70 | 3.9 |
| $^{32}$S | 0.56 | 4.4 |
| $^{36}$Ar | 0.25 | 6.6 |

We note that the alteration of the initial Hartree-Fock determinant by the replacement

$$\varphi_\alpha(\vec{r}_j) \rightarrow \exp(i\vec{k}\cdot\vec{r}_j)\varphi_\alpha(\vec{r}_j)\,, \tag{13}$$

has no effect whatsoever upon the calculated value of $\tau_D$. This results from the fact that $\tau_D$ (and $\Delta E_0$ as well) involves only the translationally invariant operations of the exact Hamiltonian, $H^{EX}$. Because of the same invariance, the determinant formed from the Hartree-Fock eigenstate by the replacement (13) evolves under TDHF dynamics as a pure translation of the eigenstate

$$\psi(t_0)=\mathcal{A}\sum_{i=1}^{A}\varphi_{x_i}(\vec{r}_i), \tag{14}$$

with velocity $\vec{v}=\hbar\vec{k}/m$, and without alteration of its intrinsic structure.

The center of interest for TDHF computer modeling is, of course, the collision of two nuclear heavy ions. Therefore, the values of $\tau_D$ for that problem are of special interest. Unfortunately, no one who has so far calculated a TDHF numerical model of nuclear heavy-ion collisions has evaluated $(\Delta E_0)^2$, expression (10), by which we were able via already published stationary-state Hartree-Fock results[5] to obtain the quantitative estimates of $\tau_D$ for an isolated nucleus given in Table I. [Indeed, one goal of the present report is to encourage practioners to include $(\Delta E_0)^2$ in their reported results.] Therefore we are only able at present to offer arguments toward the following qualitative conclusions: (a) During the early stage of a collision, the values of $\tau_D$ will be of the same order of magnitude as those in Table I, and (b) the general qualitative tendency in later stages of the collisions will be for the dependency lifetime, $\tau_D$, to grow shorter, the more energetic the process. In advancing this argument we consider for simplicity only collisions involving two identical nuclei.

For well-separated nuclei, we write the sum in (9) as three subsums,

$$\Sigma=A^{-1}\sum_{\substack{\mu\nu\in F\\ \sigma\tau\notin F}}|\bar{v}_{\mu\nu,\sigma\tau}|^2=\Sigma^{RR}+\Sigma^{LL}+\Sigma^{LR}, \tag{15}$$

in which subsums the filled states $(\mu\nu)$ are both localized in the right nucleus (RR), both in the left (LL), or one from each (LR). Then, so long as the nuclear volumes have zero spatial overlap, the terms in each of these three sums are in exact one-to-one correspondence which can be labeled by the following correspondence among the Fourier components of the single-nucleon wave functions for either nucleus at rest, for the left nucleus translating to the right with momentum $+\hbar\vec{K}$ per particle, or for the right nucleus translating toward the left with momentum $-\hbar\vec{K}$ per particle:

$$\vec{k}_\alpha{}^0 \longleftrightarrow \vec{k}_\alpha{}^L=\vec{k}_\alpha{}^0+\vec{K} \longleftrightarrow \vec{k}_\alpha{}^0=\vec{k}_\alpha{}^0-\vec{K}. \tag{16}$$

Then one obtains immediately the result

$$\Sigma^{RR}=\Sigma^{LL} \tag{17}$$

by inspection of the corresponding matrix elements. Also, if the two nuclei are separated by more than the range of the nucleon-nucleon force, every matrix element in $\Sigma^{LR}$ vanishes identically because of vanishing overlap of the factors in the integrand. Thus $\Sigma^{LR}\equiv 0$. Furthermore, when the nuclei begin to approach within the force range, the term-by-term correspondence guarantees that

$$\Sigma^{LR}=g\Sigma^{RR}, \tag{18}$$

where $g$ is a (small) geometric factor describing the average reduction of the squared matrix element which results from the (now small) spatial overlap of the folded two-body potential of one nucleus with the density of the other. Thus one concludes (even were $g$ to be as large as 1) that in the very early stages of the collision process the magnitude of $\Sigma$ (and thus of $\tau_D$) in (9) is, within a factor of 2 or so, the same for colliding ions as for isolated ions. Thus Table I is relevant also to nuclear collision processes.

To support the conclusion that the times in Table I are also relevant to nuclear heavy-ion collisions, in that they provide an upper bound for the dependency lifetimes of such processes, we

emphasize that the Pauli exclusion principle is the source of a strong tendency to keep the value of $\tau_D$ in (9) small, and that that tendency is weakened with increasing initial kinetic energy. Thus, more energetic processes promise generally smaller dependency times, $\tau_D$. In particular, although the number of filled states, and therefore of pairs $(\mu\nu)$, is fixed by the nucleon number $A(N,Z)$, the number of possible final-state pairs $(\sigma\tau)$ is reduced by the exclusion principle, as compared with the number which would otherwise be consistent with the fundamental limitations (e.g., momentum conservation and momentum transfer) of the same two-nucleon interaction. Thus, as the initial energy of the two colliding ions increases, this "Pauli" reduction factor,[6] describing the ratio of the number of allowed final states to the maximum possible number of final state, approaches unity, and the sum in (9) approaches its "Boltzmann limit"

$$\Sigma \to \Sigma_B = A^{-1} \sum_{\substack{\mu\nu \in F, \\ \text{all } \sigma,\tau}} |\bar{v}_{\mu\nu,\sigma\tau}|^2 = A^{-1} \sum_{\mu\nu \in F} (V^2)_{\mu\nu,\alpha\beta}, \quad (19)$$

in which the sum over the unfilled states is replaced by an unrestricted sum over *all* states. The dependency time, correspondingly, approaches the "Boltzmann" time

$$\tau_D \to \tau_B = 2\hbar \Sigma_B^{-1/2}, \quad (20)$$

which is always less than $\tau_D$.[7] Thus, one expects in general[8] that increased reaction energy will involve dependency times even shorter than those given in Table I.

One concludes that a natural time scale exists which raises doubt about the use of single-determinantal approximations in time-dependent quantum dynamical calculations, since the characteristic time is not so large as to guarantee easily that the TDHF dynamics will remain accurate long enough to complete the description of a nuclear heavy-ion collision. Conservative practice rather recommends that the dependence $D$ (or some similar quantity) be computed in each TDHF calculation as a figure of merit for the adequacy of that approximation to the true dynamical evolution. The fact that for zero-range forces the leading nonzero term in $D(t)$ is infinite[7] suggests that an especially cautious view of the TDHF calculations utilizing such forces is appropriate.

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[1]James J. Griffin and Peter Lichtner, in *Proceedings of the Fourth International Workshop on Gross Properties, Hirschegg, Austria, 1976,* edited by W. Myers and H. v. Groote, AED-Conf.-76-015-000 (Institut für Kernphysik, Technische Hochschule, Darmstadt, Germany), p. 21, and University of Maryland Technical Report No. 76-096, April 1976 (unpublished).

[2]P. Bonche, S. E. Koonin, and J. W. Negele, Phys. Rev. C 13, 1226 (1976); S. E. Koonin, Phys. Rev. Lett. 61B, 227 (1976); R. Y. Cusson, R. K. Smith, and J. A. Maruhn, Phys. Rev. Lett. 36, 1166 (1976).

[3]This assumption we shall always utilize in the present paper. We postpone further discussion of inaccuracies from limitations upon the initial conditions as outlined in Ref. 1 until a later report.

[4]The definition of the dependency *per particle*, via the factor $A^{-1}$ in Eq. (3), makes the dependency range, $0 \leq D < 1$, independent of $A$, and has the effect that the wave function describing two or more identical nuclei well separated in space has exactly the same value of $D(t)$ as that for one of the nuclei in isolation. A corresponding scaling then seems appropriate in Eq. (10).

[5]M. K. Banerjee, Diogenes D'Oliveira, and G. J. Stephenson, Jr., Phys. Rev. 181, 1404 (1969).

[6]The label "Pauli" here is used to identify "exclusion" effects, as distinguished from "exchange" effects. This usage is consistent with the term "Pauli break-up" proposed by B. L. Gambhir and J. J. Griffin [Phys. Rev. C 7, 590 (1973), and Phys. Lett. 50B, 407 (1974)] for use in the reaction theory of multi-nucleon projectiles, and the term "Pauli anisotropy" for corresponding effects upon angular distribution from N. Austern, Phys. Lett. 61B, 7 (1976).

[7]We note that the Boltzmann time, $\tau_B$, of Eq. (20), and as well the dependency lifetime itself in Eq. (9), diminish with the range of the two-nucleon interaction, approaching zero for the limit of a force proportional to $\delta(\vec{r}_1-\vec{r}_2)$. Thus for TDHF calculations involving zero-range forces, the present discussion suggests extreme caution, since the basic Hartree-Fock assumption is grossly inconsistent with the time-dependent Schrödinger equation of the system.

[8]These arguments tacitly omit the possibility of coherent effects. Therefore, they should not be considered as unexceptionable. Indeed, any stronger conclusion would violate the principle of commensurability proposed in Ref. 1, since one knows that for some nucleon-nucleon forces (long range), the Hartree-Fock description may be very accurate. A more stringent conclusion is therefore "commensurable" only with a theory in which the specific nature of the two-nucleon interaction provides an explicit prior condition for its validity.