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THE CONSTANT $\langle \mathcal{H} \rangle$ RESOLUTION OF TIME-DEPENDENT HARTREE-FOCK PHASE AMBIGUITY†

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ABSTRACT

The customary time-dependent Hartree-Fock problem is shown to be ambiguous up to an arbitrary function of time additive to $\mathcal{H}_{HF}$, and, consequently, up to an arbitrary time-dependent phase for the solution, $\Phi(t)$. The "constant $\langle \mathcal{H} \rangle$" phase is proposed as the best resolution of this ambiguity. It leads to the following attractive features: (a) the Time-Dependent Hartree-Fock Hamiltonian, $\mathcal{H}_{HF}$, becomes a quantity whose expectation value is equal to the average energy and hence constant in time; (b) eigenstates described exactly by determinants, have time-dependent Hartree-Fock solutions identical with the exact time-dependent solutions; (c) among all possible T.D.H.F. solutions this choice minimizes the norm of the quantity $(H - i\hbar\partial/\partial t)|\Phi\rangle$, and guarantees optimal time evolution over an infinitesimal period; (d) this choice corresponds both to the stationary value of the absolute difference between $\langle H \rangle$ and $\langle i\hbar\partial/\partial t \rangle$ and simultaneously to its absolute *minimal* value with respect to choice of the time-dependent phase. The source of the ambiguity is discussed. It lies in the time-dependent generalization of the freedom to

transform unitarily among the single-particle states of a determinant at the (physically irrelevant for stationary states) cost of altering only a factor of unit magnitude.

KEYWORD ABSTRACT

[NUCLEAR REACTIONS. Phase ambiguity in time-dependent Hartree-Fock method resolved by constant $\langle \mathcal{H} \rangle$ condition for modified Hartree-Fock Hamiltonian.]

1. CUSTOMARY TIME-DEPENDENT HARTREE-FOCK PROBLEM IS PHASE AMBIGUOUS

The variational principle[1-5] (where H is the exact Hamiltonian),

$$\delta I = \delta \int_{t_1}^{t_2} \langle \Psi | (H - i\hbar\, \partial/\partial t') | \Psi \rangle \, dt' = 0, \tag{1}$$

when restricted to single determinantal solutions, leads to the conditions[6]

$$\langle a_\sigma^+(t) a_\ell(t) \Phi(t) | H - i\hbar \partial/\partial t | \Phi(t) \rangle = 0, \quad (\ell \in F, \ \sigma \notin F), \tag{2}$$

where F is the set of single-particle states in the determinant, $\Phi(t)$. Thence the "customary" time-dependent Hartree-Fock problem[7,8-13]

$$\mathcal{H}^o_{HF}[\Phi_o(t)] | \Phi_o(t) \rangle = i\hbar | \dot{\Phi}_o(t) \rangle \tag{3}$$

in which the "customary" Hartree-Fock Hamiltonian, $\mathcal{H}^o_{HF}$, is the sum of A time-dependent single-particle Hamiltonians of the form given by Dirac.[3] In particular, $\mathcal{H}^o_{HF}$, in second quantized form, is a pure one-body operator involving no additive C-number function of time.

However, the conditions (2) are satisfied not only by solutions Φ_o of (3), but also by the solutions, Φ, of *any* equation obtained by replacing $\mathcal{H}^o_{HF}$ by

$$\mathcal{H}_{HF} = \mathcal{H}^o_{HF} + B(t) \tag{4}$$

where B(t) is an arbitrary real C-number function of time. The solutions $\Phi(t)$ and $\Phi_o(t)$ are related by

$$\Phi(t) = \Phi_o(t) \exp\{-i/\hbar \int_{t_o}^{t} dt' \, B(t')\} = \Phi_o(t) \exp\{if(t)\} \tag{5}$$

so that the freedom to choose B(t) corresponds to the freedom to select an arbitrary time-dependent C-number as a complex phase in the solution Φ. For this reason, we refer to the customary T.D.H.F. problem (in which B(t) is implicitly chosen to be zero) as "phase ambiguous."

We note (a) that the exact time-dependent Schrödinger initial value problem exhibits no such time-dependent phase ambiguity,[14] and (b) that any treatment of a time-dependent problem in which two or more wave functions are additively combined[15-18] may be affected by the time-dependent phases of those wave functions. It follows therefore that the resolution of this phase ambiguity in T.D.H.F. promises practical consequences.

The construction of the one-body density matrix, ρ, from the T.D.H.F. wave function suppresses the physical information contained in the time-dependent C-number phase of the wave function, Φ. This is evident from the fact that the resulting[3] equivalent of the T.D.H.F. equation (3),

$$i\hbar\dot{\rho} = [\mathcal{H}^{o}_{HF}, \rho], \tag{6}$$

is unaffected by a transformation of the form (4). It follows that the density matrix formulation of T.D.H.F. must "close" the description by precluding the incorporation of wave functions other than the T.D.H.F. solution into the description. Although several approximate wave functions can be combined to yield a unique density matrix, several approximate density matrices can not, unless an additional statement supplies the information carried by the (relative) time-dependent phases of the corresponding wave functions.

2. RESOLUTION OF THE T.D.H.F. PHASE AMBIGUITY FOR AN EIGENSTATE

To resolve the choice of B(t), and of f(t) in Eq. (5), consider a case where some determinant, χ_o, is the ground state eigenfunction[19] of the exact Hamiltonian, H,

$$H\chi_o = E_o\chi_o . \tag{7}$$

Then the exact solution, Ψ, of the Schrödinger time-dependent problem which reduces at $t = t_o$ to the initial value χ_o, is

$$\Psi(\vec{x};t) = \{\exp - iE_o(t - t_o)/\hbar\}\chi_o. \tag{8}$$

Since the energy of an eigenfunction is certainly stationary with respect to arbitrary variations of the wave function, χ_o must be the least energy solution of the stationary Hartree-Fock problem, and an eigenfunction of the Hartree-Fock Hamiltonian,[20]

$$\mathcal{H}^o_{HF}\chi_o = \varepsilon_o\chi_o. \tag{9}$$

In the Hartree-Fock approximation the time-dependent problem becomes

$$\{\mathcal{H}^o_{HF} + B(t)\}\Phi(\vec{x},t) = i\hbar\dot{\Phi}(\vec{x},t) \tag{10}$$

with solution

$$\Phi(\vec{x},t) = \{\exp - i/\hbar[\varepsilon_o(t - t_o) + \int_{t_o}^{t} B(t')dt']\}\Phi(\vec{x};t_o). \tag{11}$$

Then the choice

$$\int_{t_o}^{t} B(t')dt' = [E_o - \varepsilon_o] \cdot (t - t_o) \tag{12}$$

or, for the arbitrary function, B(t), the choice

$$B(t) = B(t_o) = E_o - \varepsilon_o = \langle H - \mathcal{H}^o_{HF}\rangle, \tag{13}$$

guarantees that the Hartree-Fock solution to this time-dependent problem is identically equal to the exact solution.[21,22]

3. GENERAL RESOLUTION OF PHASE AMBIGUITY: CONSTANT $\langle\mathcal{H}\rangle$ T.D.H.F.

The choice (12)-(13) for B suggests the following prescription for the general time-dependent Hartree-Fock problem:

$$B(t) = \langle\Phi(t)|(H - \mathcal{H}^o_{HF}(t))|\Phi(t)\rangle. \tag{14}$$

With this choice the T.D.H.F. problem becomes

$$[\mathcal{H}_{HF}]\Phi = [\mathcal{H}^o_{HF} + \langle H - \mathcal{H}^o_{HF}\rangle]\Phi = i\hbar\dot{\Phi}. \tag{15}$$

It is remarkable that there follows the relationship,

$$\langle \mathcal{H}_{HF} \rangle \equiv \langle H \rangle = E. \tag{16}$$

Since $\langle H \rangle$ is conserved during the T.D.H.F. evolution,[3] so is $\langle \mathcal{H}_{HF} \rangle$ for this "constant $\langle \mathcal{H} \rangle$" choice of B(t). We consider this serendipitous feature to constitute a strong recommendation for this "constant $\langle \mathcal{H} \rangle$" resolution of the ambiguity, (4).

4. MINIMIZATION OF THE ERROR NORM AMONG T.D.H.F. SOLUTIONS

A plausible alternative to (1) as variational principle for T.D.H.F. is to require that the determinant, Φ, be chosen so that the quantity

$$(H - i\hbar\partial/\partial t)|\Phi\rangle \tag{17}$$

have a minimal norm; that is, that[23]

$$I_N = \langle (H - i\hbar\partial/\partial t)\Phi(t) | (H - i\hbar\partial/\partial t)\Phi(t) \rangle \tag{18}$$

be a minimum with respect to variation of $\Phi(t)$. Unfortunately, this variational principle does not in general yield the T.D.H.F. formulation,[24,25] unless applied in an appropriately restricted subspace.[26] However, as an *auxiliary* criterion for selecting among the set of phase ambiguous T.D.H.F. formulations, (4), the condition (18) seems a reasonable optimizer. For solutions of the form (11), I_N becomes

$$I_N = \{B(t) + \frac{1}{2} \sum_{\substack{m \in F \\ n \in F}} \hat{V}_{mn;mn}\}^2 + \sum_{\substack{mn \in F \\ \sigma\tau \notin F}} |\hat{V}_{\sigma\tau;mn}|^2. \tag{19}$$

Thus, its minimization with respect to choice of B(t) selects

$$B(t) = -\frac{1}{2} \sum_{\substack{m \in F \\ n \in F}} (\hat{V}_{mn;mn}) = -\frac{1}{2} \mathcal{V}_{HF}(t), \tag{20}$$

a choice which is identically equal to that given by (13), since

$$\langle H - \mathcal{H}^{o}_{HF} \rangle = -\frac{1}{2}\mathcal{V}_{HF}(t) = -\frac{1}{2}\sum_{\substack{m\in F\\ n\in F}} \hat{V}_{mn;mn}. \tag{21}$$

5. OPTIMAL CORRESPONDENCE WITH EXACT TIME EVOLUTION FOR SHORT INTERVAL

As a final recommendation for the "constant $\langle\mathcal{H}\rangle$" T.D.H.F. formulation, we note that the exact solution specified initially by the determinant, $\Phi(\vec{x},t_o)$, can be described at $t = t_o + \Delta t$ by the Taylor series

$$\Psi(\vec{x},t) = \sum \frac{1}{n!}\left(\frac{\Delta t}{i\hbar}\right)^n (H)^n \Phi(\vec{x},t_o) \tag{22}$$

whereas the Hartree-Fock approximant is

$$\Phi(\vec{x},t) = \sum \frac{1}{n!}\left(\frac{\Delta t}{i\hbar}\right)^n (\mathcal{H}_{HF})^n \Phi(\vec{x},t_o). \tag{23}$$

The additive function B(t) in $\mathcal{H}_{HF}$ can be chosen so that the leading non-zero term (proportional to Δt) in the difference overlap,

$$\langle \Psi(\vec{x},t) \,|\, (\Psi(\vec{x},t) - \Phi(\vec{x},t)) \rangle = 0 + \frac{\Delta t}{i\hbar}\langle H - \mathcal{H}_{HF}\rangle + O[(\Delta t^2)], \tag{24}$$

vanishes. This leads again to the "constant $\langle\mathcal{H}\rangle$" choice specified by Eqs. (14), (16), and (21). For an infinitesimal time step, this is the same condition as was applied to the eigenfunction case in Sect. 2.

6. A NEW PRINCIPLE: A STATIONARY, AND MINIMAL, ABSOLUTE VALUE INTEGRAL

Besides the operational advantages already cited, the specific time-dependent Hartree-Fock Hamiltonian (15), and the corresponding choice of the time derivative, invite a reformulation of the variational basis of T.D.H.F. In particular, the quantity

$$\langle \Phi \,|\, (H - i\hbar\partial/\partial t) \,|\, \Phi \rangle = \langle \Phi \,|\, (H - \mathcal{H}_{HF}) \,|\, \Phi \rangle = 0 \tag{25}$$

vanishes identically for the choice (14). Thus, if the variational quantity (1) were replaced by its absolute value,

$$I_A = \left|\langle\Phi(t)\right|(H - i\hbar\partial/\partial t)\left|\Phi(t)\rangle\right|, \qquad (26)$$

this "constant $\langle\mathcal{H}\rangle$" choice of phase would guarantee that I_A realizes its absolute minimal value (zero). One sees therefore that the requirements that the variational quantity I_A be (a) stationary with respect to infinitesimal variations of the determinant, Φ, plus the additional condition that (b) it be minimal with respect to the time-dependent C-number phase of Φ, yields immediately the unambiguous "constant $\langle\mathcal{H}\rangle$" Hartree-Fock formulation (15), leading to the solution (11) with $\bar{B}(t')$ given by (14). Since the variational quantity (26) yields a natural basis to apply the auxiliary condition for a *minimum*, whereas principle (1) provides a continuous set of *stationary* solutions, but offers no basis whatsoever for preferring any particular one of them, the quantity (26) with the conditions (a) and (b) would appear to provide a formulation of T.D.H.F. superior to that of variational principle (1).

7. ORIGIN OF THE PHASE AMBIGUITY

Why does the T.D.H.F. system exhibit such a phase ambiguity? We note the fact, well known in stationary state Hartree-Fock theory, that an arbitrary unitary transformation among the single-particle states of a stationary Hartree-Fock determinant leads to no alteration of the physical description: *adding* to any row of a determinant any linear combination of its other rows effects no change whatsoever in the determinant, apart from a physically inconsequential constant multiplicative factor (which must, to preserve the normalization, be of unit magnitude).

In the time-dependent framework, this same property of determinants allows an arbitrary *time-dependent* unitary transformation, which leads once again to the same determinant except for a (now *time-dependent*) factor of unit

magnitude. Thus, the origin of the phase ambiguity of T.D.H.F. is seen to lie in this same property of determinants, and is therefore, a posteriori, unsurprising.[27]

8. SUMMARY AND CONCLUSIONS

The customary T.D.H.F. formulation has been shown to be phase ambiguous. A particular "constant $\langle \mathcal{H} \rangle$" specification of the arbitrary function of time which defines the phase of the T.D.H.F. solution has been suggested. Several ways in which this choice seems convenient and advantageous are noted, including a new absolute valued variational quantity whose stationary values gives the customary T.D.H.F., and whose (unique) *minimal* value corresponds to the "constant $\langle \mathcal{H} \rangle$" choice of the phase. This phase ambiguity arises from a property of determinants which trivializes in the stationary case.

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6. The time integral in (1) conforms the variational process conceptually and dimensionally with the derivation of the field equations from a Lagrangian density. However for the Hartree-Fock problem the integral leads to no practical consequence for infinitesimal variational processes. For these the condition, $d\langle\Phi|\delta\Phi\rangle/dt = 0$, is automatically fulfilled when both Φ and $\Phi + \delta\Phi$ are required to be determinants. This condition can be used to give the same results usually obtained by integration by parts under the time integral. The time integration is therefore often omitted, as in the remainder of this paper.
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14. Apart from the phase, $-C_o t/\hbar$, arising from the addition of a time-independent constant, C_o, to the Hamiltonian, which merely specifies the (arbitrary) zero of the energy scale. See also footnote 20.

15. Although most T.D.H.F. applications to date have been "closed" applications of the method, in which only the one solution occurs, certain attempts have recently been made to project or to join that solution onto sets of asymptotic wave functions in order to extract scattering or reaction information. (Cf., Ref. 16.) Also, a complete multi-wave function restructuring of the self-consistent field description of continuum process (the so-called "T.D.-$\mathcal{S}$-Matrix-H.F.") has been proposed in Refs. 17 and 18. In such descriptions the relative time-dependent phases of the several wave functions have physical content and can affect the implications of the theory.

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19. Non-trivial examples do exist. Consider, e.g., the case of A fermions enclosed in a spherical box of radius, $r_o/2$, and interacting via square well two-body potentials of range, r_o. Then each eigenstate is a deter-

minant of single-particle eigenfunctions of the spherical infinite square well potential. Thus the argument in the text is not vapid, as it might have been had the eigenfunctions of Hamiltonians with two-body interactions turned out *never* to be determinantal. If several determinantal states are eigenfunctions, then the discussion in the text applies to that determinantal eigenstate, denoted by χ_o, which has the least eigenvalue, E_o.

20. Note that the addition of any real constant, C_o, to $\mathcal{H}^o_{HF}$ does not alter this argument. Physically, such an addition simply shifts the zero of the energy scale to a new value. Indeed, we shall see below that in the generalization from stationary to time-dependent determinants, the corresponding possibility to replace such a (physically irrelevant) constant by an arbitrary function of time is the mathematical source of the phase ambiguity.

21. A different choice, corresponding to the complete elimination of the time-dependent phase in (11) is suggested in Ref. 22. There the view of T.D.H.F. is as a "closed" system in which the overall phase of the wave function is of no physical significance.

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23. Since this quantity is actually used here as an auxiliary optimizer, rather than as the variational source of the field equations, there is no compulsion to include (nor to omit) an integral over time in the definition (18) of the error to be minimized. (Cf. Eq. (1) and footnote 6.)

24. As a result, Eq. (18) cannot provide for the time-dependent Hartree-Fock formulation a *minimal* principle analogous to the Rayleigh-Rydberg-Ritz principle for the stationary Hartree-Fock problem. The contrary assertion is found in Ref. 25. On the other hand, variation of the quantity (18) with respect only to $\langle\dot{\Phi}|$ for fixed determinantal Φ does lead to the T.D.H.F. result, Eq. (2), asserted on page 59 of Ref. 25. But this procedure does not necessarily provide a *minimum* of the error (18).

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27. This freedom was noted in some early derivations of the T.D.H.F. equation (Ref. 2), and in some more recent work (Ref. 22), but without the recognition that it might be exploited to theoretical advantage in multi-wave function descriptions.