PHYSICAL REVIEW C VOLUME 21, NUMBER 5 MAY 1980

Alternative methods for the solution of static Hartree-Fock and related problems

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(Received 30 July 1979)

Alternative ways to the usual diagonalization procedures to solve the self-consistent nuclear Hartree-Fock problem are discussed. It is shown that they are much faster than the conventional approach and computationally much simpler. It is shown how they can be further improved. Finally all these new methods are unified within the framework of a direct minimization of the total energy in the subspace of Slater determinants. Results are given for medium-light deformed nuclei.

[NUCLEAR STRUCTURE Alternative Hartree-Fock solutions.]

I. INTRODUCTION

Certainly the Hartree-Fock (HF) approximation represents a starting point for any microscopic attempt to describe nuclear structure. In addition, with the introduction of schematic density-dependent interactions, this approach has recently shown its validity in reproducing static ground state properties of a wide range of nuclei.[1] Constrained HF calculations, coupled to an evaluation of the collective mass parameter in an adiabatic time evolution, seem to give very promising results in describing large amplitude oscillations far away from the stability region (fission modes, yrast states, and so on).[1] Therefore it seems worthwhile to improve the numerical methods for solving the HF problem in order to obtain faster convergence and more reliable solutions, particularly for the case of heavy deformed nuclei.

The usual approach is based on a linearization of the HF equation which leads to a self-consistent diagonalization of the HF Hamiltonian

$$h_F(\rho)=T+\mathrm{Tr}\tilde{V}\rho+\tfrac{1}{2}\,\mathrm{Tr}\,\mathrm{Tr}\,\rho\frac{\partial\tilde{V}}{\partial\rho}\rho\,, \tag{1.1}$$

where T is the kinetic energy $\tilde{V}$ is the antisymmetrized interaction, and ρ is the one-body density matrix of the nuclear system. The third term has to be included when one uses density-dependent forces.

The diagonalization method is actually a quite lengthy procedure for heavy elements where huge matrices are involved. On the other hand this approach is based on a particular linearization of a problem which is highly nonlinear, especially for density-dependent interactions. This means that a different linearization can lead to much faster convergence. Finally, the reduction of the problem to the solution of a Schrödinger equation raises some mathematical uncertainties in constrained cases because of the unboundedness which occurs for certain values of the Lagrange multipliers in the Hamiltonian.[2,3]

Recently two methods have been proposed to overcome such difficulties which make no use of diagonalization procedures. One, the "direct density" approach, is based on a minimization of the total energy through a steepest descent procedure in the space of one-body density matrices.[4] The other, the "imaginary time" approach, is based on a transformation of single particle wave functions which resembles a time evolution with imaginary time and which ensures a decreasing total energy towards the minimum value.[5]

In this paper we show that the two approaches are closely related in a general framework of a direct minimization problem for the total energy functional with different linearization options which lead to different convergence rates, also connected to the density dependence of the used schematic interaction. We shall focus our attention on the HF problem, but the extension of these methods and of our conclusions to constrained cases and to the Hartree-Fock-Bogoliubov problem is straightforward.[6]

II. DIRECT ENERGY MINIMIZATION METHOD

Here we briefly discuss the method, and demonstrate the possibility of including higher order terms in the variation of the energy functional with respect to the density matrix. The problem is to minimize the total energy in the HF approximation

$$E(\rho)=\mathrm{Tr}T\rho+\tfrac{1}{2}\,\mathrm{Tr}\,\mathrm{Tr}\rho\tilde{V}\rho \tag{2.1}$$

in the space of the one-body density matrices with the constraints

$$\begin{aligned} &\rho^\dagger = \rho\,, \\ &\rho^2 = \rho\,, \\ &\mathrm{Tr}\rho = A\,. \end{aligned} \tag{2.2}$$

This means that if we start with a density matrix ρ_0 which satisfies the HF conditions [Eqs. (2.2)] and if we operate with a unitary transformation

$$\rho = e^{i\chi}\rho_0 e^{-i\chi}\,, \tag{2.3}$$

our problem reduces to a search for an Hermitian operator χ which secures a maximum energy decrease at each step.

We can introduce an expansion for the energy variation

$$\Delta E = \left\langle \frac{\partial E}{\partial \rho} \middle| \Delta\rho \right\rangle + \frac{1}{2}\left\langle \frac{\partial^2 E}{\partial \rho^2}\cdot\Delta\rho \middle| \Delta\rho \right\rangle + \frac{1}{6}\left\langle \left(\frac{\partial^3 E}{\partial \rho^3}\cdot\Delta\rho\right)\cdot\Delta\rho \middle| \Delta\rho \right\rangle + \cdots \tag{2.4}$$

in a matrix space with scalar product

$$A\cdot B = \langle A|B\rangle \equiv \mathrm{Tr}A^{+}B\,. \tag{2.5}$$

Because of the very general result

$$\frac{\partial E}{\partial \rho} = h_F(\rho)\,, \tag{2.6}$$

where $h_F(\rho)$ is the HF Hamiltonian, Eq. (2.4) may be rewritten as

$$\begin{aligned} \Delta E &= \mathrm{Tr}\left[h_F(\rho) + \frac{1}{2}\,\frac{\partial h_F}{\partial \rho}\cdot\Delta\rho + \frac{1}{6}\left(\frac{\partial^2 h_F}{\partial \rho^2}\cdot\Delta\rho\right)\cdot(\Delta\rho)\right]\Delta\rho + \cdots \\ &\equiv \mathrm{Tr}h_{\mathrm{eff}}(\rho)\Delta\rho + \cdots\,. \end{aligned} \tag{2.7}$$

We remark that no further terms are needed for linearly density-dependent forces (e.g., of Skyrme type). In any case, we have a definite way to consider higher order terms.

Assuming the trial density matrix ρ_0 is not far away from the solution, we can approximate

$$\delta\rho \sim i\,[\chi, \rho_0]\,. \tag{2.8}$$

We finally get

$$\Delta E = -i\,\mathrm{Tr}[h_{\mathrm{eff}}, \rho_0]\chi \tag{2.9}$$

and the choice[4]

$$\chi = i\lambda[h_{\mathrm{eff}}, \rho_0]\,, \tag{2.10}$$

with λ real positive, ensures a maximum energy decrease of the truncated energy at each step. The result is actually related to the approximation equation (2.8). In this respect the choice of the λ parameters requires some attention. In order to secure the validity of the approximation equation (2.8), where we neglect higher order terms in the χ operator, we must keep

$$\|\chi_n\| \ll 1\,, \quad n = 0, 1, \ldots\,.$$

In our metric this means

$$\lambda_n \ll \frac{1}{\|[h_{\mathrm{eff}}^{(n)}, \rho_n]\|} = \frac{1}{(-\mathrm{Tr}[h_{\mathrm{eff}}^{(n)}, \rho_n]^2)^{1/2}}\,, \tag{2.11}$$

which implies a large range of acceptable values if we start with a density matrix corresponding to a good trial mean field. Actually we have no problems in nuclear theory where spherical potentials, with standard choices of depth and radius, give the bulk of the self-consistent field. In any case, from the inequality equation (2.11) it seems to be safe to choose small values of λ. A good prescription is to take the smallest real positive solution of the nonlinear equation

$$\frac{\partial E[\rho(\lambda)]}{\partial \lambda} = 0\,. \tag{2.12}$$

Expanding $\rho(\lambda)$ to the second order in λ we get a definite expression for the best value of λ (see Appendix A)

$$\lambda_{\mathrm{opt}}^{(n)} = \frac{\mathrm{Tr}(D_n{}^2)}{\mathrm{Tr}\{[D_n, h_{\mathrm{eff}}^{(n)}][D_n, \rho_n]\}}\,, \tag{2.13}$$

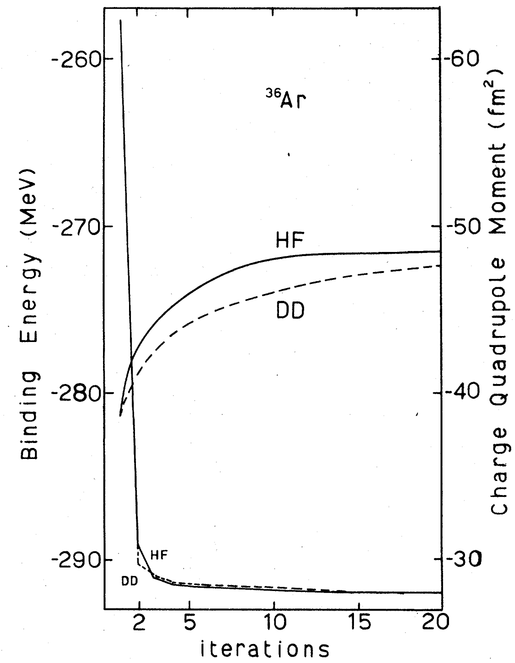

FIG. 1. Total energy (lower curves) and charge quadrupole moment (upper curves) of ^{36}Ar as a function of iteration number. HF lines are obtained with the usual procedure, DD lines refer to the method described in the text with the approximation equation (2.14).

where $D_n \equiv [h_{\mathrm{eff}}^{(n)}, \rho_n]$, with ρ_n the density matrix at the nth iteration. The approach has been proven successful for a quite wide choice of the starting density ρ_0.

In Fig. 1 we show results of this method compared to the usual HF diagonalization procedure for the energy and quadrupole moment of the ground state of ^{36}Ar. In effecting the comparison, we have used the simple DD approximation

$$h_{\mathrm{eff}}(\rho) \simeq h_F(\rho)\,, \tag{2.14}$$

i.e., we have neglected higher order terms in the energy variation ("direct density" method of Ref. 4). The interaction used is of Skyrme II type. The starting density matrix ρ_0 is computed from a spherical Woods-Saxon potential with radius $R = 1.35\,A^{1/3}$ fm, diffuseness $a = 0.6$ fm, and depth $V = -70$ MeV.[4,7] The DD method seems to be slower than standard HF, but this is not a serious difficulty because it is computationally much faster.

The introduction of second and third order terms, with a Skyrme force, significantly improves the convergence rate. This can be seen in Figs. 2, 3, and 4 for the ^{20}Ne and ^{24}Mg cases (DDH curves), where a suitable extrapolation has been used to compute the shift (see Appendix B)

$$\Delta\rho = \rho_{n+1} - \rho_n\,. \tag{2.15}$$

All the results have been obtained with a deformed harmonic oscillator basis,[7] but of course the method is not dependent on the choice of the representation.

In contrast to the HF case, both the binding energy and the charge quadrupole moment converge at about the same iteration in the DDH method. In terms of computation time the DD and DDH methods are very similar (the former being fractionally faster) because of the two intermediate estimates of the density being required in the DDH case. However, the DDH method is much more stable since an almost simultaneous convergence of the binding energy and the nuclear shape is obtained. Moreover, the DDH method is about a factor 4 faster than the usual HF.

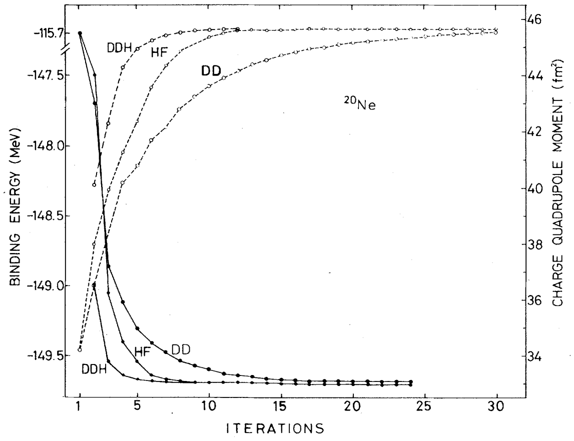

FIG. 2. Total energy (lower curves) and charge quadrupole moment (upper curves) of ^{20}Ne as a function of iteration number. The DDH lines correspond to the inclusion of higher order terms.

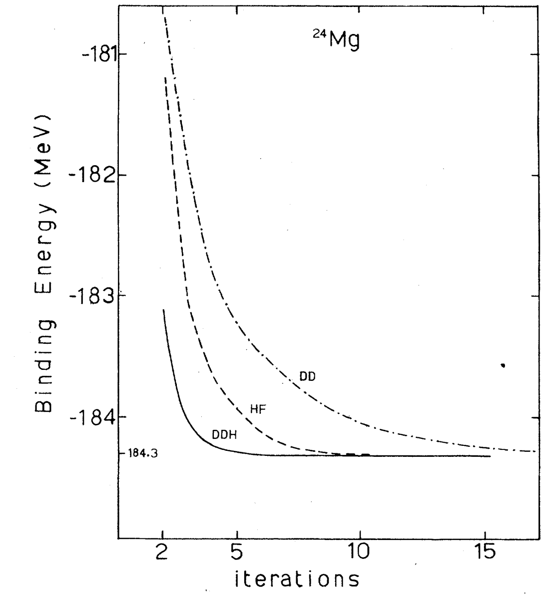

FIG. 3. Total energy of ^{24}Mg as a function of iteration number with also the results obtained with higher order terms (DDH line).

At the end of this section we would like to make two more points which are important in order to

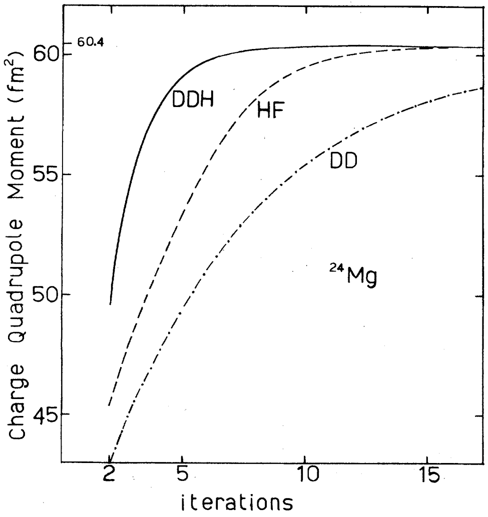

FIG. 4. The same as Fig. 2 for the charge quadrupole moment.

make connection with the imaginary time method described in the next paragraph. First of all, let us consider the changes of the single particle wave functions during the iteration procedure. If we introduce at each step the eigenstates of the one-body density matrix

$$\rho_n = \sum_i^{1,A} |\psi_i^{(n)}\rangle\langle\psi_i^{(n)}| , \qquad (2.16)$$

with the same unitary transformation as discussed previously, we can construct the eigenstates of the $(n+1)$st density matrix

$$\begin{aligned} |\psi_i^{(n+1)}\rangle &= \exp(i\chi^{(n)})|\psi_i^{(n)}\rangle \\ &= \exp\{-\lambda[h_{\text{eff}}^{(n)},\rho_n]\}|\psi_i^{(n)}\rangle . \end{aligned} \qquad (2.17)$$

Moreover, while we do not keep track of the single particle energies, which have no direct physical meaning, we can easily compute the variation of the total energy at each iteration

$$E^{n+1} - E^n \equiv \Delta E = -\lambda\,\mathrm{Tr}(D_n D_n^+) , \qquad (2.18)$$

with D_n defined in Eq. (2.13).

III. IMAGINARY TIME APPROACH

This method has been originally introduced as a byproduct of time-dependent–Hartree-Fock (TDHF) calculations and it is actually based on an "evolution" method similar to that used to describe a real time-evolving system.[5]

In the "true" TDHF we have a unitary transformation acting on single particle wave functions

$$|\psi_j^{(n+1)}\rangle = U|\psi_j^{(n)}\rangle , \qquad (3.1)$$

with

$$U = \exp\left(-i\,\frac{\Delta t}{\hbar}\,h^{(n+1/2)}\right) , \qquad (3.2)$$

where $h^{(n+1/2)}$ is an effective Hamiltonian chosen to conserve exactly the total energy in a real evolution (Appendix B of Ref. 5).

Introducing imaginary time intervals

$$\Delta T \to -i\Delta t \qquad (3.3)$$

and a suitable orthonormalization of the single particle wave functions after every "time" step, we get a fast convergence to the static solution, provided we make a "small" choice of the magnitude of Δt, actually chosen on empirical grounds. This can be clearly seen from the total energy variation shown in Eqs. (3.6)–(3.8).

From a first order expansion of the U operator we can get a precise idea of the connection with the previously described "direct energy minimization method."

At the first order we act on the single particle wave function with an operator which has the form $[1-\mu h^{(n+1/2)}]$ with $\mu = \Delta t/\hbar$ a real positive parameter. If we add the orthonormalization procedure, we finish with the transformation,[8] valid for small values of μ only,

$$\begin{aligned} |\psi_j^{(n+1)}\rangle &= (1-\mu h^{(n+1/2)})|\psi_j^{(n)}\rangle \\ &\quad + \mu\sum_k^{1,A}\langle\psi_k^{(n)}|h^{(n+1/2)}|\psi_j^{(n)}\rangle|\psi_k^{(n)}\rangle , \end{aligned} \qquad (3.4)$$

that in the density matrix formalism becomes

$$|\psi_j^{(n+1)}\rangle = [1-\mu(1-\rho_n)h^{(n+1/2)}]|\psi_j^{(n)}\rangle . \qquad (3.5)$$

On the other hand, the variation of the total energy at each iteration step is given by[8]

$$\begin{aligned} E^{(n+1)} - E^{(n)} &= \sum_j^{1,A}(\langle\psi_j^{(n+1)}|h^{(n+1/2)}|\psi_j^{(n+1)}\rangle \\ &\qquad - \langle\psi_j^{(n)}|h^{(n+1/2)}|\psi_j^{(n)}\rangle) \\ &= -2\mu\,\mathrm{Tr}(AA^+) \leqslant 0 , \end{aligned} \qquad (3.6)$$

with

$$A \equiv \rho_n h^{(n+1/2)}(1-\rho_n) . \qquad (3.7)$$

The result is a nonpositive definite variation which goes to zero at convergence, where

$$A = 0 \text{ and hence } [h^{(n+1/2)},\rho_n] = 0 . \qquad (3.8)$$

IV. CONNECTION BETWEEN THE TWO APPROACHES

It is easy to show that we obtain very similar results, in fact identical in form, within the direct energy minimization (DEM) framework. Indeed the first order expansion of the unitary transformation equation (2.17) gives

$$|\psi_j^{n+1}\rangle \simeq [1-\lambda(1-\rho_n)h_{\text{eff}}]|\psi_j^n\rangle . \qquad (4.1)$$

For the total energy variation we get from Eq. (2.18), using the cyclic property of the trace and the idempotency $\rho_n{}^2 = \rho_n$,

$$E^{n+1} - E^n = \Delta E = -2\lambda\,\mathrm{Tr}(BB^+) \leqslant 0 , \qquad (4.2)$$

where

$$B = \rho_n h_{\text{eff}}(1-\rho_n) , \qquad (4.3)$$

so that at convergence

$$[h_{\text{eff}}(\rho_n),\rho_n] = 0 . \qquad (4.4)$$

If we compare Eqs. (4.1), (4.2), and (4.4) with the relations (3.5), (3.6), and (3.8) we see a striking similarity between the two approaches. The similarity can be strengthened by demonstrating the equivalence of the Hamiltonians $h^{(n+1/2)}$ and h_{eff}, as we now show for the case with the simplified density-dependent two-body interaction,[5]

$$v_2 = t_0\delta(\vec{r}_1-\vec{r}_2) + \frac{t_3}{6}\rho\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)\delta(\vec{r}_1-\vec{r}_2) , \qquad (4.5)$$

with which imaginary time calculations have been extensively done.

Now the Hartree-Fock Hamiltonian becomes

$$h_F^{(n)} = -\frac{\hbar^2}{2m}\Delta + \tfrac{3}{4} t_0 \rho_n + \tfrac{3}{16} t_3 \rho_n^2 , \tag{4.6}$$

where ρ_n is the *local* density at the *n*th iteration. In Ref. 5 it is shown that in this case the $h^{n+1/2}$ operator to be used in the imaginary time-step formalism is given by

$$h^{n+1/2} = \tfrac{1}{2}(h_F^{(n)} + h_F^{(n+1)}) - \frac{t_3}{32}(\rho_{n+1} - \rho_n)^2 . \tag{4.7}$$

We can compare now with the h_{eff} operator used in the DEM method

$$h_{\text{eff}}^{(n)} = h_F^{(n)} + \frac{1}{2}\frac{\partial h_F^{(n)}}{\partial \rho}\cdot \Delta\rho + \frac{1}{2}\frac{\partial^2 h_F^{(n)}}{\partial^2 \rho}\cdot(\Delta\rho)^2 . \tag{4.8}$$

Because the HF Hamiltonian now is a function of the local density only, and introducing

$$\Delta\rho = \rho_{n+1} - \rho_n ,$$

we get

$$\begin{aligned} h_{\text{eff}} &= h_F^{(n)} + \tfrac{1}{2}(\tfrac{3}{4} t_0 + \tfrac{3}{8} t_3 \rho_n)(\rho_{n+1} - \rho_n) \\ &\quad + \tfrac{1}{16} t_3 (\rho_{n+1} - \rho_n)^2 \\ &= \tfrac{1}{2}(h_F^{(n)} + h_F^{(n+1)}) - \frac{t_3}{32}(\rho_{n+1} - \rho_n)^2 \\ &= h^{(n+1/2)} . \end{aligned} \tag{4.9}$$

The two Hamiltonians are exactly the same, order by order, in the density shift $\Delta\rho$. Indeed we can easily show that the term $\frac{1}{16} t_3(\rho_{n+1} - \rho_n)^2$ in $h^{n+1/2}$ comes from third order contributions in $\Delta\rho$ to the total energy variation.[5] Actually if we expand

$$\begin{aligned} \rho_{n+1}{}^3 &= \rho_n{}^3 + \Delta\rho(\rho_{n+1}{}^2 + \rho_n \rho_{n+1} + \rho_n{}^2) \\ &= \rho_n{}^3 + \Delta\rho[3\rho_n\rho_{n+1} + (\rho_{n+1} - \rho_n)^2] \\ &= \rho_n{}^3 + 3\rho_n\rho_{n+1}\Delta\rho + (\Delta\rho)^3 \end{aligned} \tag{4.10}$$

and if we neglect $(\Delta\rho)^3$ terms in the variation $E^{n+1} - E^n$, we get again a relation [Eq. (3.2)] with a

$$h^{(n+1/2)} = h_F^{(n)} + \tfrac{1}{2}(\tfrac{3}{4} t_0 + \tfrac{3}{8} t_3 \rho_n)(\rho_{n+1} - \rho_n) , \tag{4.11}$$

i.e., with a second order h_{eff} only.

In conclusion we can say that there is a perfect equivalence between the two methods in the limit of small values of λ. However, we remark that in the DEM approach we are not bound to choose very small values of this parameter, the only condition being Eq. (2.11), which can allow a wide range of choices. Moreover, we get a definite prescription for finding the best parameter λ at each iteration step [see Eq. (2.12)]. All that, as expected from general grounds, can improve the velocity of convergence. However, we must remark that there is a "numerical" price to pay: at each iteration we need the construction of the whole density matrix.

We would like to close this section with a remark related to the empirical observation[9] of obtaining a faster convergence using an average HF Hamiltonian

$$h_{\text{AV}} = \tfrac{1}{2}(h_F^{(n)} + h_F^{(n+1)}) \tag{4.12}$$

in the conventional HF method, with density independent interactions. In this case, which corresponds to $t_3 = 0$, the operator h_{eff} is just the average Eq. (4.12), as can be clearly seen from Eq. (4.9). This means that one is actually solving the equation

$$[h_{\text{eff}}(\rho), \rho] = 0 ,$$

which, from the previous analysis, corresponds to a minimization of the total energy with a better linearization procedure.

V. CONCLUSION

In this paper we showed that the "direct density" (DD or DDH) and the imaginary time approaches to solve static HF problems can be seen as two sides of a general method based on a direct minimization of the total energy in the space of the one-body density matrices.

Many advantages can follow from this connection and in general from the development of nondiagonalizing procedures to solve HF-type problems:

(i) We have now available methods which are much faster than the conventional HF procedures. In addition, for axially symmetric nuclei, charge quadrupole moments and binding energies are found to converge simultaneously at about the same iteration.

(ii) We have a definite way to generalize the approach to any density-dependent nuclear interaction.

(iii) We can get a precise prescription on the choice of the length of the "time step" following Eq. (2.12).

(iv) We can easily extend the method to the Hartree-Fock-Bogoliubov problem, which can be seen as a minimum problem for the energy functional in a generalized density matrix space.[6]

(v) In this framework of a general minimum problem we can make use of several mathematical tools to study constrained situations (shape, angular momentum, and so on).

ACKNOWLEDGMENTS

We are grateful to D. M. Brink, H. Flocard, and D. Vautherin for helpful suggestions and useful discussions. F. D. would like to thank Professor R. Vinh Mau for his kind hospitality at Orsay and the CNRS for a research fellowship. The work of

M. D. T. and G. R. was supported in part by INFN, Sezione di Catania, and by CSFNSM.

APPENDIX A: SEARCH FOR THE BEST λ

With our choice of the χ operator [Eq. (2.10)] the λ-dependence of the density matrix is given by

$$\begin{aligned}\rho_{n+1}^{(\lambda)} &= e^{-\lambda D_n}\rho_n e^{\lambda D_n}\\ &= \rho_n - \lambda[D_n, \rho_n] + \frac{\lambda^2}{2}[D_n, [D_n, \rho_n]]\\ &\quad - \frac{\lambda^3}{6}[D_n, [D_n, [D_n, \rho_n]]] + \cdots\end{aligned}$$

with

$$D_n = [h_{\text{eff}}^{(n)}, \rho_n] .$$

Neglecting third order terms, the variation with respect to λ is

$$\Delta\rho = \frac{\partial\rho}{\partial\lambda}\Delta\lambda \simeq -[D_n, \rho_n]\Delta\lambda + \lambda[D_n, [D_n, \rho_n]]\Delta\lambda .$$

Our nonlinear equation (2.12) becomes

$$\begin{aligned}\frac{\Delta E}{\Delta\lambda} &= \mathrm{Tr}\, h_{\text{eff}}^{(n)} \frac{\Delta\rho}{\Delta\lambda}\\ &\simeq \mathrm{Tr}\, h_{\text{eff}}^{(n)}\{-[D_n, \rho_n] + \lambda[D_n[D_n, \rho_n]]\} = 0 ,\end{aligned}$$

with solution

$$\lambda_{\text{opt}}^{(n)} = \frac{\mathrm{Tr}(D_n{}^2)}{\mathrm{Tr}\{[D_n, h_{\text{eff}}^{(n)}][D_n, \rho_n]\}} > 0 , \tag{A2}$$

which can be shown to be positive in the region of validity of the whole method.

We can easily consider higher order terms in Eq. (A1). In this way we get higher order equations in λ. The prescription is to choose the smallest real positive solution. Condition equation (A2) ensures the existence of a solution of this kind.

APPENDIX B: EXTRAPOLATION OF THE DENSITY MATRIX

Since h_{eff}^{n} is dependent on $\Delta\rho = \rho_{n+1} - \rho_n$ we must evaluate the $(n+1)$-th density matrix through some extrapolation procedure. We can follow several ways to do it (Lagrangian, exponential, and also linear), always obtaining convergence rates faster than HF.

We get the best results, reported as DDH curves in Figs. 2, 3, and 4 using a more involved predictor-corrector method. $\Delta\rho$ is estimated introducing successively higher order terms during each iteration as follows:

$$\begin{aligned}&\rho_n \to h_F(\rho_n) \to \rho_{n+1}^{(0)} \to h_F(\rho_n) + \tfrac{1}{2}h_F'(\rho_n)(\rho_{n+1}^{(0)} - \rho_n)\\ &\quad \to \rho_{n+1}^{(1)} \to h_F(\rho_n) + \tfrac{1}{2}h_F'(\rho_{n+1}^{(1)} - \rho_n)\\ &\quad\quad + \tfrac{1}{6}h_F''(\rho_n)(\rho_{n+1}^{(1)} - \rho_n) \to \rho_{n+1} .\end{aligned}$$

Thus we make two intermediate guesses $\rho_{n+1}^{(0)}$ and $\rho_{n+1}^{(1)}$ for the new density matrix before obtaining its best evaluation ρ_{n+1} .

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