A Time-Dependent Multi-Determinant approach to nuclear dynamics.

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Abstract

We propose a Time-Dependent Multi-Determinant approach to the description of the time evolution of the nuclear wave functions (TDMD). We use the Dirac variational principle to derive the equations of motion using as ansatz for the nuclear wave function a linear combination of Slater determinants. We prove explicitly that the norm and the energy of the wave function are conserved during the time evolution. This approach is a generalization of the time-dependent Hartree-Fock method to many Slater determinants. We apply this approach to a case study of $^6$Li using the N3LO interaction renormalized to 4 major harmonic oscillator shells. We solve the TDMD equations of motion using Krylov subspace methods of Lanczos type. As an application, we discuss the isoscalar monopole strength function.

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1 Introduction.

The time-dependent Hartree-Fock method (TDHF) and its quasi-particle generalization, the time dependent Hartree-Fock-Bogoliubov method (TDHFB), are central tools in studying nuclear dynamics (see for example ref. [1], ref. [2] for a recent review and references in there). In these approaches the time dependence of the nuclear wave function is studied under the assumption that the nuclear wave function can be described by a single Slater determinant or by a quasi-particle determinant wave function. Usually nuclear excitations, for example giant resonances, are studied in the approximation of small amplitude motion around the static solution (RPA or QRPA). In this case, the description of nuclear excitations reduces to the solution of a large eigenvalue problem. Despite the enormous matrix dimensions, the RPA or QRPA equations are solved nowadays using efficient Krylov projection techniques of Arnoldi type (see for example ref.[3] for recent applications). Recently, the time-dependent coupled-cluster method (refs. [4],[5]) has been revisited (ref. [6]) and it has been applied to light nuclei (ref.[7]) using the N3LO interaction (ref. [8]) transformed by the similarity renormalization group.

In this work we discuss a Time-Dependent Multi-Determinant (TDMD) approach whereby the nuclear wave function is approximated by a linear combination of several Slater determinants. This approach is the time dependent version of the Hybrid Multi-Determinant (HMD) approach (refs. [9]-[11]). Each Slater determinant is built from different single-particle wave functions of the most generic type. To the author knowledge, this approach has never been considered in nuclear physics. In this sense, this is an exploratory study. Our starting point is the Dirac variational principle which, as well known, leads to the time-
dependent Schroedinger equation in the most general case, or to the TDHF equations (ref.[12]) if the nuclear wave function is approximated by a single Slater determinant. Using the Dirac variational principle, we derive the equations of motion and prove explicitly that the time evolution conserves the norm and the energy of the wave function. The equations of motion for the single-particle wave functions are of the type $iL\dot{\psi} = R$ where $R$ is an energy gradient, $\psi$ is the set of single-particle wave functions of all Slater determinants, and $L$ is a matrix of large dimension related to the time derivative of the norm of the wave function (which will be discussed in detail below). The actual evaluation of the wave function as a function of time is performed using the Direct Lanczos method (DL) for the solution of a large linear system. The DL method belongs to the family of Krylov subspace methods for the solution of linear systems (an excellent review of these methods can be found for example in ref. [13]). These methods for eigenvalue problems include the familiar Lanczos method used in the shell model approach to nuclear structure (refs. [14],[15]) and the Arnoldi method used in solving the RPA or QRPA eigenvalue problems (ref.[3]). The basic idea of these methods is the following. Although we may not be able to store a matrix (e.g. the nuclear Hamiltonian matrix) we can easily evaluate the matrix to vector product. In our case, although $L$ is not as large as the shell model Hamiltonian matrix, it can hardly be stored except in simple cases. However the matrix to vector product appearing in the equations of motion is trivial to evaluate, and the Lanczos method is the ideal one. We solve the equations of motion, as an exploratory study, in the case of $^6Li$ using the N3LO interaction renormalized to 4 major oscillator shells with the Lee-Suzuki (ref.[16],[17]) method, in order to reduce the otherwise very large single-particle space. We use the time-dependent wave function obtained in
this way to evaluate strength functions. Our ultimate goal is to extend ab-initio
methods to time-dependent problems, such as the evaluation of strength functions,
starting from a two-body nucleon-nucleon interaction.

Our approach is different from the Multiconfiguration Time-Dependent Hartree
(or Hartree-Fock) method (MCTDHF) used in quantum chemistry (ref. [18]-[20]).
The MCTDHF is a time dependent version of the shell model written in the full
Hilbert space. The MCTDHF method uses a time-dependent linear combination
of all possible Slater determinants. The time-dependent coefficient of such a lin-
ear combination is a function of all possible many-body configurations and it is
obtained using the equations of motion. Since the ansatz for the many-body wave
function is not unique, one restricts the freedom in the many-body wave function
by imposing orthogonality among the single-particle wave functions. As shown
in ref. [19] this amounts to a redefinition of the coefficient of the linear combi-
nation. The only difference between an exact treatment of the time evolution of
the many-body wave function and the MCTDHF approach is that in the latter the
single-particle basis is time dependent. In the MCTDHF approach, at a given
value of time, all Slater determinants are built from the same time-dependent
single-particle basis, that is, each of them is a n-particle-n-hole excitation from
the lowest one. In our approach, instead, each Slater determinant is built from a
different time-dependent single-particle basis. Moreover, we consider several and
not all possible Slater determinants and we do not have the freedom of imposing
orthogonality between the single-particle wave functions belonging to different
Slater determinants. Rather, we consider the most generic Slater determinants, in
the same spirit of the HMD method. Our approach is not limited by the dimen-
sion of the Hilbert space. Each Slater determinant, in our approach, is equivalent
to a rather large number of linear combinations of the Slater determinants of the MCTDHF approach. As a consequence, the equations of motion in the MCTDHF approach are different from the ones of the TDMD approach (cf. ref. [18]-[20] and section 2a of this work).

The outline of this paper is as follows. In section 2 we derive the equations of motion in the TDMD approach using the Dirac variational principle, we prove that these equations of motion conserve the norm and the energy of the nuclear wave function and discuss how to fix uniquely the solution of the equations of motion for the single-particle wave functions. We also briefly discuss the imaginary time version of these equations of motion. At the end of section 2 we discuss the 'static' solutions of these equations and show that the time propagation of these solutions generates a time-dependent phase factor common to all Slater determinants (in some sense this is the generalization of the single-particle energies). In section 3 we discuss the numerical method and in section 4 we discuss the application of our method to the nuclear strength function using the boost method in order to determine the excitation spectrum.

2 The time-dependent variational principle.

2a. Equations of motion and conservation laws.

The Dirac time-dependent variational principle states that the time evolution of the nuclear wave function is obtained by varying the action

\[ S_1 = \int_{t_1}^{t_2} dt \mathcal{L}_1 = \int_{t_1}^{t_2} dt \left[ i \hbar < \psi | \dot{\psi} > - < \psi | \hat{H} | \psi > \right] \]  

(1a)
or equivalently

\[
S_2 = \int_{t_1}^{t_2} dt \mathcal{L}_2 = \int_{t_1}^{t_2} dt \left[ -i\hbar \dot{\psi} |\psi\rangle - <\psi|\hat{H}|\psi\rangle \right]
\]  

(1b)

with respect to $|\psi\rangle$ and $<\psi|$ independently, under the constraint that the wave function is held fixed at the initial and final times $t_1$ and $t_2$. The use of the most general wave function in the Hilbert space reproduces the Schrodinger equation and its complex conjugate. The TDHF approximation is obtained if the wave function is approximated by one Slater determinant. In what follows we drop $\hbar$ with the understanding that the unit of time is $1\text{MeV}^{-1} \approx 6.6 \times 10^{-22}\text{sec}$. We consider the following ansatz for the nuclear wave function

\[
|\psi\rangle = \sum_{S=1}^{N_w} |U_S\rangle
\]  

(2)

where $|U_S\rangle$ is a Slater determinant and $N_w$ is their number. These Slater determinants for $A$ particles are of the most generic type and are written as

\[
|U_S\rangle = c_{1S}^\dagger c_{2S}^\dagger \ldots c_{AS}^\dagger |0\rangle
\]  

(3)

$A$ being the number of particles, $S$ labels the Slater determinant and

\[
c_{\alpha S}^\dagger = \sum_{i=1,N_s} U_{i,\alpha S} a_{i}^\dagger, \quad (\alpha = 1, 2, \ldots, A)
\]  

(4)

in the above equation, $a_i^\dagger$ is the creation operator in the single-particle (e.g. harmonic oscillator) state $i$, $N_s$ is the number of the single-particle states and $U$ is the single-particle wave function in the h.o. representation. Note that these single-particle wave functions are different for each Slater determinant labeled by the index $S$. In what follows we label particles with greek letters and single-particle states with latin letters.

As mentioned in the introduction, in the MCTDHF (cf. ref.[20]) each Slater determinant is written as a multi-particle multi-hole excitation built on the first
one. Moreover in the MCTDHF approach it is essential to multiply each Slater determinant by a time-dependent amplitude and the time-dependent single-particle states can be taken orthogonal to each other. That is, in the MCTDHF approach,

\[ |\psi > = \sum_{n_1, n_2, \ldots} A(n_1, n_2, \ldots, t)|n_1, n_2, \ldots t >, \]

with the sum extending over all possible allowed values of the occupation numbers of the time-dependent basis, i.e. \( n_1, n_2, \ldots = 0, 1 \). These considerations illustrate the basic difference between the TDMD approach proposed in this work and the MCTDHF approach.

We assume that each Slater determinant is a product of a neutron and a proton Slater determinant. The ansatz (3)-(4) is the same of the Hybrid multi-determinant method (refs.[9]-[11]) used in variational calculations. Usually in the HMD method, a projector to good quantum numbers (angular momentum and parity) is applied to the wave function of eq.(2), in order to decrease the otherwise large number of Slater determinants needed to obtain accurate energies, for example for the yrast states. In this work, we do not use projectors to good quantum numbers. We do this in order to simplify the equations and the proof of the conservation of the energy and of the norm. The Slater determinants are not orthogonal to each other and are 'deformed', that is, they do not have good quantum numbers. At the initial time they could be the result of a partially converged variational calculation as given by the HMD method, or converged variational wave functions 'boosted' by some excitation operator (e.g. dipole, quadrupole, etc.). We do not have the freedom to impose the orthogonality between the single-particle wave functions belonging to different Slater determinants, although we can impose orthogonality between the single-particle wave functions of the same Slater determinants.

Although the Dirac variational principle determines uniquely the time dependence of the Slater determinants, it does not uniquely fix the single-particle wave
functions $U_{\alpha S}$. In order to see this, let us perform the following transformation of the generalized creation operators defined in eqs. (3) and (4).

$$c_{\alpha S}^{\dagger} = \sum_{\beta=1}^{A} g_{\alpha,\beta}(S)c_{\beta S}^{\dagger} \quad (\alpha = 1, 2, \ldots, A)$$

(5)

for every $S$. In other words, we mix the particle labels in each Slater determinant, but we do not mix the particle labels of different Slater determinants. Each Slater determinant can be rewritten as

$$|U(S) > = \det(g(S))c_{1S}^{\dagger}c_{2S}^{\dagger} \ldots c_{AS}^{\dagger}|0 >$$

(6)

Therefore, provided $\det(g(S)) = 1$, the same Slater determinant can be obtained using the new generalized creation operators

$$c_{\alpha S}^{\dagger'} = \sum_{i} a_{i}U_{i\alpha S}$$

(7)

with, in matrix notation,

$$U'(S) = U(S)\tilde{g}(S)^{-1}$$

(8)

Hence, if the $U$’s are a solution of the equations of motion (discussed below) also the $U'$ given by equation (8) with any $g$ (provided $\det(g) = 1$), will satisfy the same equations of motion. This kind of gauge invariance implies that the equations of motion, although they determine the time evolution of the set of Slater determinants, they do not determine unambiguously the time evolution of the single-particle wave functions $U(S)$. Since $g$ is arbitrary (provided $\det(g) = 1$), we have $A^2 - 1$ free parameters for each Slater determinant. In order to uniquely specify the solutions of the equations of motion we select the matrix $g$ such that

$$U'_{\alpha\beta} = \text{diag}(1, 1, \ldots, U'_{AA})_{\alpha\beta} \quad (\alpha, \beta = 1, 2, \ldots, A)$$

(9)

for the $A \times A$ submatrix of $U$ for each Slater determinant. In eq. (9), $U'_{AA}$ is the determinant of the $A \times A$ submatrix of $U$. This point will be further discussed after
the equations of motion have been derived. We assume that all Slater determinants have been recast so that the $A \times A$ submatrices of the single-particle wave functions are as in eq.(9) and in what follows we shall drop the prime. In this way we effectively decrease the number of unknowns.

We now proceed to determine the equations of motion of the single-particle wave functions $U$. In what follows, since we always have pairs of indices $S$ and $S'$, the Slater determinant $|U_S>$ will have the label $S$ (even though sometimes it will be omitted) and the the complex conjugates of $|U_{S'}>$, $<0|c_{AS'}...c_{1S'}$, where

$$c_{\alpha,S'} = \sum_i V_{\alpha,iS'} a_i$$

will have the label $S'$. $V_{S'}$ is the Hermitian conjugate of the matrix $U_{S'}$. We do this in order to use simple matrix notations, and to avoid confusion between $U$ and $U^\dagger$ for different $S$ and $S'$ since often we omit the labels $S$ and $S'$ in order to shorten the equations. The Dirac variational principle gives (the bra will be denoted as $<V|$)

$$i \sum_S \delta_{V(S')} <V_S|\dot{U}_S> = \delta_{V(S')} \sum_S <V_S|\hat{H}|U_S>$$  \hspace{1cm} (11a)

$$-i \sum_{S'} \delta_{U(S)} <V_{S'}|U_S> = \delta_{U(S)} \sum_{S'} <V_{S'}|\hat{H}|U_S>$$  \hspace{1cm} (11b)

where we have shown explicitly the quantities which are varied. In what follows, we quote the results for the overlaps and for the matrix elements of the Hamiltonian (cf. ref.[9]). The Hamiltonian is

$$\hat{H} = \frac{1}{2} \sum_{ijkl} H_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$$

where we recast the one-body term into the two-body interaction, as done in shell model calculations. The matrix elements of $H$ are antisymmetrized (i.e. $H_{ijkl} = -H_{ijlk}$). For any $V$ and $U$, (relative to the Slater determinants $S'$ and $S$
respectively) let us define

\[ G = (V U)^{-1}, \quad W = G V, \quad X = U G, \quad \rho = U G V, \quad F = 1 - \rho \]  

(13)

The matrix \( G \) has indices \( \alpha, \beta = 1, 2, \ldots, A \). The matrix \( W \) has indices \( \alpha, i \), the matrix \( X \) has indices \( i, \alpha \) while \( \rho \) and \( F \) have indices \( i, j = 1, 2, \ldots, N_s \). The matrix \( \rho \) is the generalization of the density matrix in TDHF and satisfies the relations \( \text{tr} \rho = A \) and \( \rho^2 = \rho \) for any \( S' \) and \( S \), as it can easily be verified. We have then (cf. ref.[9])

\[ <V|U> = \det(VU) \]  

(14)

\[ <V|\hat{H}|U> = <V|U> \text{tr}(\Gamma \rho) \]  

(15)

where the matrix \( \Gamma \) is given by

\[ \Gamma_{ij} = \sum_{pq} H_{pqij} \rho_{qp} \]  

(16)

Let us note that the exchange term is the same of the direct since the matrix elements are antisymmetrized. The equations of motion eqs.(11a),(11b) (EOM1 and EOM2) can be derived using the matrix identity, for any matrix \( M \),

\[ \delta \det(M) = \det(M) \text{tr}(M^{-1} \delta M) \]  

(17)

Then it is easy to verify that

\[ <V|\dot{U}> = <V|U> \text{tr}(GV\dot{U}) \]  

(18a)

\[ <\dot{V}|U> = <V|U> \text{tr}(GVU) \]  

(18b)

and that the explicit form for EOM1 is (using the identity \( \delta M^{-1} = -M^{-1} \delta MM^{-1} \))

\[ i \sum_{r\mu,S} \det(VU)(X_{ia} W_{ir} + F_{ir} G_{\mu a}) U_{r\mu S} = \sum_S \det(VU)(X_{ia} \mathcal{E} + 2(FTX)_{ia}) \]

(19)
where $\mathcal{E}$ is the energy functional

$$\mathcal{E} = \text{tr}(\Gamma \rho)$$

(20)

The equation of motion EOM2 can be obtained in the same way and is given by

$$-i \sum_{\mu,r,S} \det(VU)(W_{\alpha i}X_{\tau \mu} + G_{\alpha \mu}F_{\tau i}) \dot{V}_{\mu r S} = \sum_{S'} \det(VU)(\mathcal{E}W_{\alpha i} + 2(W \Gamma F)_{\alpha i})$$

(21)

These equations need a few comments. First, if we recast them in a schematic matrix notation

$$iL^{(1)} \dot{U} = R^{(1)}$$

(22a)

$$-iL^{(2)} \dot{V} = R^{(2)}$$

(22b)

the dimension of the linear systems to be solved can be rather large. For example, in the case of $^{24}\text{Mg}$ with 7 major shells ($N_s = 168$) for 10 Slater determinants, the matrix $L$ is $20160 \times 20160$ (for both neutrons and protons), for a larger number of major shells or for heavier nuclei, the storage of this array in the computer memory can be a problem. Moreover these matrices seem to have some kind of separable structure. $L^{(1)}$ for example contains a separable term in the indices $(i\alpha)(\mu r)$ and another separable term in the $(i r)(\mu \alpha)$ indices. This implies that although we may not be able to store the matrix $L$, we can very easily perform the matrix to vector product. We only needs to store the matrices $X, W, F$ and $G$, in the case of $^{24}\text{Mg}$, of dimension $168 \times 12, 12 \times 168$ and $168 \times 168$ for every $S$ and $S'$. These matrices are the same matrices used in the HMD variational calculations. In the past few decades, linear systems of this type, for which the matrix cannot be stored but the matrix to vector product can easily be performed, have received a major attention in applied mathematics using the so called Krylov subspace techniques. These techniques are precisely of the same kind one uses in standard shell
model calculations (ref.[13]). They will be briefly recalled in the next section. A systematic treatment can be found in ref. [13] (note however that in ref. [13] the convention for the scalar product is \( < x | y > = \sum x_i y_i^* \)). Equations of motion EOM1 and EOM2 are equivalent. The matrix \( L^{(1)} \) and \( L^{(2)} \) are Hermitian.

One can show that the norm of the wave function is preserved during the time evolution, using the explicit form of the equations of motion. From eqs. (14) and (17) one has

\[
d < \psi | \psi > / dt = \sum_{SS'} < V | U > tr[ G (\dot{V}U + V\dot{U})] \tag{23}
\]

with the understanding that \( S' \) refers to \( V \) and \( S \) to \( U \). From EOM1 eq. (19), multiplying by \( V_\alpha S' \) and summing over the indices one has

\[
i \sum_{SS'} < V | U > [ tr(\rho)tr(GVU) + tr(F\dot{U}G) ] = \sum_{SS'} < V | U > [ tr(\rho)\mathcal{E} + 2tr(\rho \Gamma F) ] \tag{24}
\]

From EOM2 of eq. (21), multiplying by \( U_\alpha S \) and summing over the indices one has

\[
-i \sum_{SS'} < V | U > [ tr(\rho)tr(G\dot{VU} + XV\dot{F}) ] = \sum_{SS'} < V | U > [ tr(\rho)\mathcal{E} + 2tr(\rho \Gamma F) ] \tag{25}
\]

Subtracting eqs. (24) and (25), and since for any \( SS' \), \( tr(\rho) = A \), we have

\[
i \sum_{SS'} < V | U > [ A tr[G(\dot{V}U + V\dot{U})] + tr(F\dot{U}W + X\dot{V}F) ] = \sum_{SS'} < V | U > 2tr(F\Gamma \rho - \rho \Gamma F) \tag{26}
\]

The right hand side of this equation is 0 since \( F = 1 - \rho \). Next, since \( tr(\dot{\rho}) = 0 \) for any \( S'S \), using the definition of \( \rho \) given in eq.(13) and the cyclic property of the trace, we have

\[
tr[G(\dot{V}F U + VF\dot{U})] = 0 \tag{27}
\]
This equation can also be verified directly using the definitions in eq. (13). Hence from eq.(26), using the cyclic property of the trace, one has

\[ i \sum_{SS'} <V|U> \text{tr}[G(\dot{V}U + V\dot{U})] = 0 \] (28)

which is the time derivative of the norm (cf. eq.(23)). Next we shall prove that the energy is constant during the time evolution. We need to prove that

\[ d <\psi|\dot{H}|\psi>/dt = 0 \] (29)

since the norm of the wave function is a constant. Let us set

\[ \mathcal{H}[V,U] = <\psi|\dot{H}|\psi>, \quad \mathcal{O}[V,U] = <\psi|\psi> \] (30)

The Lagrangian associated to EOM1 can be rewritten as

\[ \mathcal{L}_1 = i \sum_a \frac{\partial \mathcal{O}}{\partial U_a} \dot{U}_a - \mathcal{H} \] (31)

where \( a = (i\alpha S') \) for brevity. EOM1 can then be written as

\[ i \sum_a \frac{\partial^2 \mathcal{O}}{\partial V_b \partial U_a} \dot{U}_a = \frac{\partial \mathcal{H}}{\partial V_b} \] (32)

for all \( b = (\beta j S') \). Similarly the Lagrangian associated with EOM2 can be recast as

\[ \mathcal{L}_2 = -i \sum_b \frac{\partial \mathcal{O}}{\partial V_b} \dot{V}_b - \mathcal{H} \] (33)

and EOM2 can be recast as

\[ -i \sum_b \frac{\partial^2 \mathcal{O}}{\partial V_b \partial U_a} \dot{V}_b = \frac{\partial \mathcal{H}}{\partial U_a} \] (34)

Multiplying eq.(32) by \( \dot{V}_b \) and summing over the indices, and similarly multiplying eq.(34) by \( \dot{U}_a \) and summing over indices, after subtracting the two results, we obtain

\[ \sum_a \frac{\partial \mathcal{H}}{\partial U_a} \dot{U}_a + \sum_b \frac{\partial \mathcal{H}}{\partial V_b} \dot{V}_b = 0 \] (35)
which is precisely the time derivative of $\mathcal{H}$. These two constants of motion are a valuable test to check whether the equations of motion have been integrated with reasonable accuracy.

Before leaving this subsection, let us discuss the consequence of the fact that the physical objects are the Slater determinants, rather than the single-particle wave function. Without fixing $A^2 - 1$ coefficients for each Slater determinant, we would have an infinite number of solutions for the linear system of eq.(19) or eq.(21) in the unknowns $\dot{U}$ or $\dot{V}$. This implies that $\det(L) = 0$ and that a direct attempt to solve the equations of motion by matrix inversion will fail. We must first fix $A^2 - 1$ coefficients for each Slater determinant before any attempt to use direct methods (such as Gaussian elimination) to solve the linear system. This means that we can consider all $\dot{U}_{\alpha,\beta} = 0$ for $\alpha, \beta = 1, \ldots, A$, except $\alpha = \beta = A$, and reduce the dimension of the linear system accordingly. The condition of eq.(9) is not equivalent to orthogonality of the single-particle wave functions (even for the same Slater determinant). We find eq.(9) simpler to implement for several Slater determinants than the orthogonality, as shown by the structure of the equations of motion. Only in the case of a single Slater determinant they can be made orthogonal and orthogonality is preserved during the time evolution. All these considerations have been tested numerically. We did not find any need to enforce eq. (9) using Krylov subspace techniques. Actually all initial calculations have been performed without the gauge fixing condition of eq.(9). Note also that if we impose (for a given $S$) orthogonality between the single-particle wave functions we would have to introduce Lagrange multipliers, while the condition of eq.(9), simply reduces the number of unknowns in the linear system of eq.(19).

2b. Imaginary time equations of motion.
Propagation in imaginary time can be used to determine the best approximation to the ground-state for a specified number of Slater determinants. As \( \tau = it \to \infty \) we obtain the ground-state of the system. We solve the following imaginary time equations of motion

\[
L \dot{V} = -R
\]  

(36)

where \( L \) and \( R \) are given in the previous subsection in eq. (21). We consider EOM2 since the basic matrices in eq.(13) can be taken from HMD computer programs, which have accurately been tested. We also solve the variational problem using the HMD method (which is a quasi-newtonian method). The technical details of the variational methods used in the HMD approach can be found in ref. [21]. The results from the HMD method can be used as initial start in eq. (36) and vice versa. We obtain the same energies from the two methods and this is a strong validation test of our computer programs. Once \( \dot{V} \) in eq. (36) has be found, we determine \( V \) using Runge-Kutta methods with a time interval sufficiently small so that the energy decreases as a function of the imaginary time. Typical values for the imaginary time interval are \( 10^{-2}, 10^{-3} \, MeV^{-1} \).

2c. The static solutions.

Let us suppose that we have found the ground state wave function for a selected number of Slater determinants, either by imaginary time propagation or with the variational HMD method, and let us call these single-particle wave functions \( \overline{V}(S') \). As in the the TDHF approximation, we can propagate in real time these static single-particle wave functions and obtain the single-particle energies. However, in the case of several Slater determinants we cannot define the single-particle energies since we do not have a self-consistent eigenvalue problem as in the HF approximation. The question naturally arises whether one can define
some type of single-particle energies from the evolution of the static solutions \( V(S) \). In the case of several Slater determinants, since we do not impose orthogonality between single-particle wave functions, these can mix. Hence we seek solutions of the type

\[
V_{\alpha iS'}(t) = \sum_{\beta=1}^{A} f_{\alpha\beta}(t, S') V_{\beta iS'}
\]

with the \( A \times A \) matrix \( f \) determined by the equations of motion EOM2. The matrices \( U, X, W, G, \rho, \Gamma \) and \( F \) for a pair of Slater determinants \( S, S' \) obey the relations, in a matrix notation,

\[
U(S) = \overline{U}(s)f^{-1}(t, S), \quad G = f^{-1}(t, S)\overline{G}f^{-1}(t, S')
\]

\[
W = f^{-1}(t, S)\overline{W}, \quad X = \overline{X}f^{-1}(t, S'), \quad \rho = \overline{\rho}
\]

\[
E = \overline{E}, \quad F = \overline{F}, \quad \Gamma = \overline{\Gamma}
\]

Quantities with the overline are obtained with the imaginary time propagation or with the HMD method. The equation EOM2 then gives

\[
\sum_{S'} \det(VU) \det(f(t, S'))[W\text{tr}(XM) + GF] = \sum_{S'} \det(VU) \det(f(t, S'))[EW + 2WF]
\]

where

\[
M = -i f^{-1}(t, S') \dot{f}(t, S')
\]

We seek time-independent \( M \) i.e. \( f = \exp(iMt) \). Since eq.(39) has to be valid at all times \( \det(f(t, S')) \) must be independent of \( S' \), i.e. all Slater determinants must evolve with the same phase factor \( \exp[itr(M)t] \). As a consequence the Fourier decomposition of the wave function gives an energy \( E_{FT} = \text{tr}(M) \). Generally, this spectral energy differs from the energy obtained from the variational calculation. However, the two energies must converge to the same value if we consider
a sufficiently large number of Slater determinants so that the exact wave function is sufficiently well approximated. This considerations must be kept in mind when we extract energies using spectral decomposition of the wave functions. In general one can define the following spectral density of a Hamiltonian $\hat{H}$ relative to some state $|\phi_0>$$$
abla(E) = <\phi_0| \delta(E - \hat{H}) |\phi_0> = \sum_n |<\phi_0|n>|^2 \delta(E - E_n) \tag{41}$$ where $E_n$ are the energies for the eigenstates $|n>$. The spectral density can be obtained from the Fourier transform of the time correlation function $<\phi_0|\phi(t)>$, where $|\phi(t)>$ is obtained from the time evolution of the initial state $|\phi_0>$, as $$\rho(E) = \frac{1}{\pi} \text{Re} \lim_{\Gamma \to 0^+} \int_0^\infty e^{i(E + \Gamma)t} <\phi_0|\phi(t)> \tag{42}$$ The number of the Slater determinants has to be sufficiently large for this method to be reliable. Moreover, if the initial state is the static solution of the imaginary time evolution, we would obtain only one pole corresponding to $E = \text{tr}(M)$, which is obviously wrong in the HF case. Hence eq. (42) gives reasonable estimates for the eigenvalues only if there is reasonable fragmentation of $\rho(E)$ for a sufficiently large number of Slater determinants. Moreover, for this method to be reliable one has to show that the spectrum obtained in this way, is independent of the initial wave function $|\phi_0>$. In this work we will not study the convergence properties of this method. We prefer to obtain the static energies using variational methods or by imaginary time propagation since we obtain upper bounds for the energy, while the energies obtained with eq. (42) are not upper bounds to the exact values.

As discussed in the next sections in the context of the boost method for strength functions, we need static solutions to a high degree of accuracy. The reason is the
The expectation values of a one-body operator \( Q = a_i^\dagger q_j a_j \) are given by

\[
< \psi(t)|Q|\psi(t) > = \sum_{S,S'} \det(VU) \text{tr}(\rho q)
\]

In the static limit, since neither the determinant nor \( \rho \) change in time, \( < \psi(t)|Q|\psi(t) > \) is constant. This is strictly true if we have determined the exact variational wave function. A small error in these wave functions can give rise to a spurious time dependence in the expectation values. However, the purpose of the boost method is to perturb slightly the variational wave function with a boost of the type \( e^{i\eta Q} \), for small values of \( \eta \), and to analyze the time dependence of the expectation values of \( Q \) in order to obtain the strength function. We found that very small changes in the energies of the ground state as we proceed in the variational calculation, is not a good criterion. We prefer to use the fact that one-body observables should not change during the real time evolution if we have determined the static solution with sufficient accuracy. This problem is hardly seen for a small number of Slater determinants since in these cases it is not difficult to determine the static solutions with the necessary accuracy. This criterion is essential, especially for small values of \( \eta \).

3 A brief description of the numerical method.

We solve numerically EOM2 (eq.21) and eq.(22b)) for \( \dot{V} \). As pointed out in the previous section, it is not advisable to store the matrix \( L_2 \). However we can easily evaluate \( L_2 v \) where \( v \) is any vector. Actually, we can easily evaluate any power of \( L_2 \) applied to \( v \). The linear system of eq.(22b) can be solved by projecting
eq.(22b) into the subspace (known as Krylov subspace) generated by the vectors $v, L_2v, (L_2)^2v, \ldots$, where $v$ is an arbitrary trial solution of the linear system, followed by Gram-Schmidt orthonormalization. Since $L_2$ is Hermitian, its projection in the Krylov subspace gives a tridiagonal matrix (just as in the shell model method) and the linear system can then be efficiently solved. We have implemented the so called direct Lanczos method, the full detail of which (including the algorithm) can be found in ref. [13]. With this method the tridiagonal linear system is solved efficiently. In our computer program the iterations stop when the residual vector $-i L_2 \dot{V} - R_2$ has a norm less than $10^{-7} \div 10^{-11}$. The dimension of the Krylov subspace is less than the dimension of the linear system of eq.(22b) and, although it is advisable to implement eq.(9), we found no actual need.

In this work we considered $^6Li$ with the interaction given by the N3LO nucleon-nucleon potential renormalized using the Lee-Suzuki method to 4 major harmonic oscillator shells. We considered $\hbar \omega = 12\, MeV$ and we added to the Hamiltonian the center of mass Hamiltonian $\beta(P_{cm}^2/2mA + mA\omega R_{cm}^2/2 - 3\hbar \omega/2)$ with $\beta = 1$. The ground-state energies in MeV’s as a function of the number of Slater determinants are the following: $E(N_w = 1) = -15.933$, $E(N_w = 15) = -22.911$, $E(N_w = 25) = -24.033$. Without using projectors to good quantum numbers, the absolute values of the energies converge slowly as a function of the number of Slater determinants. For $N_w = 200$, re-projecting the wave functions to good angular momentum and parity we obtained $E_{gs} = -28.672$. Since for large $N_w$ we have $E(N_w) \approx E_0 + const/N_w$ we can extract an extrapolated ground state energy of $-28.774$.

Once $\dot{V}$ has been determined, we solve the differential equation in time using a rank-4 Runge-Kutta method. The time step used in the real time evolution is
Figure 1: Variation of the energy (in MeV) and variation of the norm as a function of time. We took 3 Slater determinants with 4 major shells at $\hbar \omega = 12 MeV$. Snapshots are taken every $0.5 MeV^{-1}$. Typically $10^{-3} \div 10^{-4} MeV^{-1}$. In fig. 1 we show the errors in the energies and in the overlaps $DE = E(t) - E(0)$ and $DO = \ln(O(t)/O(0))$ as a function of the real time.

In fig. 1 we took snapshots every 500 time steps. Typically we ran the time evolution up to $\approx 50 \div 100 MeV^{-1}$. The number of Lanczos iterations needed to converge depends on the number of Slater determinants. For 1 Slater determinant (TDHF) we need about 4 Lanczos iterations to reach machine accuracy. This number increases as we increase the number of Slater determinants. For example for 3 Slater determinants we need typically 36 Lanczos iterations and for 5 Slater determinants we need about 50 iterations. We perform only a spo-
radical check of the energy of the center of mass in order to ensure that the wave function does not develop spurious center of mass excitations. We verified that \( E_{cm}(t) \approx 3\hbar \omega / 2 \). Before leaving this section, let us make a few comments about the computer implementation of the method. In exact arithmetic, the Lanczos method will generate an orthogonal basis. With finite numerical accuracy, orthogonality is lost, preventing numerical convergence. Hence it is very important to re-orthogonalize the Krylov basis, as done in the shell model method. Let us briefly recall that if we have \( n \) orthonormal vectors \(|v_1>,...,|v_n>\) and we wish to add to this set another orthogonal vector \(|v_{n+1}>\) starting from a vector \(|u>\) we can use the so called classical Gram-Schmidt method, that is we evaluate \(|u' >= |u> - \sum |v_k><v_k|u>\). In this case the scalar products \(<v_k|u>\) for \( k = 1,..,n \) can be evaluated independently using different processors. This classical Gram-Schmidt method however is known to be numerically unstable for a large number of vectors. This instability can however be cured by first orthogonalizing \(|u>\) to \(|v_1>\), then the result is orthogonalized to \(|v_2>\) and so on. This latter method is known as the modified Gram-Schmidt method and it is numerically stable. In this case, however, we cannot evaluate the several scalar products using different processors, since it is a sequential chain of calculations. The instability of the classical Gram-Schmidt method can be bypassed by simply repeating two or three times the orthogonalization procedure. We have implemented both the iterated classical and the modified Gram-Schmidt re-orthogonalization in the direct Lanczos method.
4 Strength functions.

We evaluate the strength function for a one body operator $\hat{Q}$

$$S(E) = \sum_n | < n | \hat{Q} | 0 > |^2 \delta(E - E_n^*)$$

(44)

$E_n^*$ being the excitation energy of the n-th eigenstate, with the boost method, as follows. First we determine the ground-state of the system $|0 >$, then at time $t = 0^+$ we boost the system with the unitary operator

$$| \psi(0^+) = \exp(i \eta \hat{Q}) | 0 >$$

(45)

where $\hat{Q}$ is a one-body operator. For sufficiently small values of the parameter $\eta$, only linear terms in $\eta$ can be retained. We then evolve this wave function in time by solving the equations of motion EOM2 and evaluate

$$Q(t) = < \psi(t) | \hat{Q} | \psi(t) > - < \psi(0^+) | \hat{Q} | \psi(0^+) >$$

(46)

The strength function can then be obtained using the Fourier transform of $Q(t)$ (see for example ref. [22])

$$\overline{Q}(E) = \int_0^T dt e^{i(E + i \Gamma)t} Q(t)$$

(47)

for sufficiently large $T$ such that $e^{-\Gamma T}$ is negligible via the relation

$$S(E) = \frac{1}{\eta \pi} Im(\overline{Q}(E))$$

(48)

Alternative methods for the determination of strength functions can be found in ref. [23] and in ref. [24].

In eqs. (45) and (46) the ground-state is replaced by the static solution evaluated with high accuracy. Only in this case we can safely guarantee that the response of eq.(46) is proportional to $\eta$. 

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Figure 2: Monopole strength function for $N_{w} = 1$ (TDHF).
Figure 3: Magnification of fig. 2.
The width $\Gamma$ is small and such that very high frequency oscillations in the Fourier transform are smoothed out. Typically we take $\Gamma = 0.1\text{MeV}$ since we would like to resolve also discrete levels. If we are interested only in giant resonances we can afford much larger values. We need to evolve the system after the boost for about $T = 50 \div 100\text{MeV}^{-1}$. In these exploratory calculations we have used the isoscalar monopole operator $Q = r^2$.

In figs. (2) and (3) we show the results obtained in the case of one Slater determinant (TDHF). Fig (3) is a magnification of fig (2). The strength function is dominated by the dominant peak at $E \simeq 17.8\text{MeV}$. Some weaker peaks can be seen at $E \simeq 0.1\text{MeV}$, $E \simeq 7.56\text{MeV}$ and $E \simeq 27.6\text{MeV}$.

With 2 Slater determinants we obtained the results shown in figs. (4) and (5). The
Figure 5: Magnification of fig. 4.
Figure 6: Strength function for $N_w = 3$ Slater determinants.
Figure 7: Magnification of fig. 6.
dominant peak is now at \( E \simeq 16.2\,\text{MeV} \). The secondary maxima are at \( E \simeq 0.1\,\text{MeV}, 7.5\,\text{MeV}, 27.8\,\text{MeV} \), almost on the same position of the TDHF case.

With 3 Slater determinants, we obtained the results of figs. (6) and (7). The main peak at \( E \simeq 16.7\,\text{MeV} \) shows considerable fragmentation around 15 MeV while the secondary peak at \( 7.5\,\text{MeV} \) is nearly unchanged. The peak around 27 MeV has nearly disappeared and has moved to lower excitation energies. Similar plots, using 5 Slater determinants, are shown in figs. (8) and (9). We also considered a larger number of Slater determinants, although for smaller values of \( T \), \( N_w = 15 \) and \( N_w = 25 \). In these latter cases, some high frequency oscillations still remain.

The results for the strength functions are shown in figs. (10) and (11). Note that the structure of the strength function has changed considerably, pointing out to the
Figure 9: Magnification of fig. 8.
need to consider a larger number of Slater determinants.

We have not studied the strength function for a larger number of major shells and as a function of the harmonic oscillator frequency for increasing number of Slater determinants. Such a study is necessary in order to promote the TDMD method as an ab-initio method. The Lee-Suzuki renormalization method in harmonic oscillator space gives a Hamiltonian which depends on the number of particles, on the number of major harmonic oscillator shells and on the harmonic oscillator frequency. Therefore it is a priori difficult to guess what would be the effect on the strength function of a larger number of harmonic oscillator shells and a larger number of Slater determinants. As we increase the number of major shells, the interaction becomes "harder" at short distances and we expect, on
Figure 11: Strength function for $N_w = 25$ Slater determinants.
general grounds, to need an increasing number of Slater determinants. More-
over, giant resonances lie in the continuum and, for a proper description of their
width we need a large single-particle space. Differently stated, if we select large
single-particle basis the interaction becomes stronger. Part of these problems can
be alleviated using low momentum interactions, whereby the NN interaction is
renormalized in momentum space and does not depend on the number of oscillat-
tor shells (cf. for example ref. [25] and references in there). Moreover, we expect
on general grounds that large values of the harmonic oscillator frequency would
give peaks further apart. Small values of $\bar{h}\Omega$ should give a better approximation to
the continuum giving a smaller distance among the peaks of the strength function.
To some extent, a simple remedy to the lack of the continuum is to increase the
width $\Gamma$.

In fig. 12 we compare the monopole strength functions for $N_w = 1, 25, 35$
evaluated with $\Gamma = 3 MeV$. This comparison gives an idea, although with low
energy resolution, of the degree of convergence as we increase the number of
Slater determinants. Some discrepancy between $N_w = 25$ and $N_w = 35$ still
remains, but the shapes are very similar. The TDHF result, instead, is different.
A possible cause of the discrepancy between the TDHF strength and the ones for
$N_w = 25$ and $N_w = 35$ is the angular momentum content of the wave functions. In
this work we did not project the wave functions to good angular momentum. Since
the Slater determinants break rotational symmetry we do not expect that the wave
functions to have good angular momentum, especially for a small number of Slater
determinants. We have checked the expectation values of $J^2$ for $N_w = 1, 25, 35$.
The results are the following: $< J^2 >_{N_w=1} = 6.94$, $< J^2 >_{N_w=25} = 4.54$ and
$< J^2 >_{N_w=35} = 4.21$, instead of the exact value $< J^2 > = 2$. Let us recall that
Figure 12: Low resolution strength functions for $N_w = 1, 25, 35$, for $\Gamma = 3\, MeV$. 
we are probing the system with a scalar probe. In the TDHF case, the initial wave function contains too many spurious components which are excited by the monopole probe. For large numbers of Slater determinants these are smaller and the monopole strengths are very similar.

Although we do not have a formal proof, if we have a very large number of Slater determinants, it is reasonable to assume that the number of static solutions is equal to the dimension of the Hilbert space. The number of peaks in the strength function is equal to number of static solutions that can be connected by the excitation operator to the ground-state. Unfortunately we do not know the number of static solutions of the type of eq.(3) for a given \( N_w \). In the derivation of the boost method it is tacitly assumed that the static solutions are eigenstates of the Hamiltonian.

For some recent works that take into account the continuum in the TDHF and in the TDHFB approximations, see for example refs. [26],[27]. Our main goal in this work is to define the time dependent method, solve the equations of motion and verify our computer programs. More applications will be presented in future works.

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