Extension of the Time-Dependent Multi-Determinant approach to propagators.

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Abstract

We extend the recently proposed Time-Dependent Multi-Determinant approach (ref.[1]) to the description of fermionic propagators. The method hinges on equations of motion obtained using variational principles of Dirac type. In particular we study the trace of real and imaginary time propagators, i.e. the partition function. The method is equally applicable with or without projectors to good quantum numbers. We discuss as a numerical example the micro-canonical level density obtained from the propagation in real time.

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1 Introduction.

In a recent work we introduced the Time-Dependent Multi-Determinant approach (ref.[1]) (TDMD), whereby the nuclear wave function is described as a linear combination of several Slater determinants. The Dirac variational principle has been used to obtain the equations of motion describing the time evolution of the nuclear wave function from an initial state. The method has been applied to the description of monopole resonances in a light nucleus. The TDMD has been shown to be a good dynamical approach in the sense that the initial energy and norm of the wave function are preserved by the equations of motion. In ref. [1] this has been shown without explicit reference to projectors to good quantum numbers (i.e. angular momentum and parity). The proof of norm and energy conservation can be carried out also using projectors to good quantum numbers with only minor additional algebra on the assumption that the Hamiltonian is rotational and parity invariant. The formalism of ref. [1] also has been used for imaginary time propagation which can be used to refine the ground state from an initial wave function. The purpose of this work is to extend the formalism introduced in ref. [1] to the description of quantum mechanical propagators. The key ideas are the following.

In ref. [1] the nuclear wave function is described as

\[ |\psi> = \sum_{S=1}^{N_w} |U_S> \] (1)

where \(|U_S>\) is a Slater determinant labeled by the index \(S\) and each Slater determinant was written as

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

\(A\) being the number of particles, \(S\) labels the Slater determinant and

\[ c_{\alpha S}^\dagger = \sum_{i=1,N_s} U_{i,\alpha S} a_i^\dagger, \quad (\alpha = 1, 2, \ldots, A) \] (3)
are generalized creation operators written as a linear combination of the standard creation operators $a_i^\dagger$ in the single-particle state $i$ (for example harmonic oscillator single-particle states). We can conveniently recast each Slater determinant as

$$|U_S > = \hat{U}(S) a_1^\dagger a_2^\dagger ... a_A^\dagger |0 >$$

(4)

where $\hat{U}(S)$ is an operator of the type

$$\hat{U}(S) = \exp[a^\dagger u(S) a]$$

(5)

We use here a matrix notation, that is $a^\dagger u(S) a = \sum_{ij} a_i^\dagger u_{ij}(S) a_j$, where the sum runs over the single-particle states in the basis. We call the propagators of eq.(5) elementary propagators (EP). The relation between the single-particle wave functions $U(S)$ and the matrix $u(S)$ is given by

$$U = \exp(u)$$

(6)

Note that the matrix $u$ uniquely specifies the single-particle wave functions $U$, but the inverse statement is not true. In fact, in order to construct $U$ we need all matrix elements of the matrix $u$, but only the matrix elements $U_{i,\alpha}$ for $i = 1, 2, ..., N_s$ and $\alpha = 1, 2, ..., A$ are used in eq.(3). That is, only part of the information contained in $u$ is used in the TDMD approach. We can state that

$$|\psi > = [\sum_{S=1}^{N_w} \hat{U}(S)] a_1^\dagger a_2^\dagger ... a_A^\dagger |0 >$$

(7)

The sum in the square brackets is a propagator and the wave function is obtained by projecting this propagator onto a reference state. Most of the information contained in the propagator is not used in the TDMD approach. It is natural to ask what is the equation of motion for this propagator and what kind of information can be extracted from it. We consider the following variational principles. If $\rho$ a
propagator for a Hamiltonian $H$, the propagator satisfies the following variational principles for real time,

\[ i \text{Tr} [\delta \rho^\dagger \dot{\rho}] = \text{Tr} [\delta \rho^\dagger H \rho] \]  

(8a)

\[ -i \text{Tr} [\dot{\rho}^\dagger \delta \rho] = \text{Tr} [\rho^\dagger H \delta \rho] \]  

(8b)

and for imaginary time

\[ \text{Tr} [\delta \rho^\dagger \dot{\rho}] = -\text{Tr} [\delta \rho^\dagger H \rho] \]  

(9a)

\[ \text{Tr} [\dot{\rho}^\dagger \delta \rho] = -\text{Tr} [\rho^\dagger H \delta \rho] \]  

(9b)

Eqs. (8a) and (9a) are called EOM1, and eqs. (8b) and (9b) are called EOM2. It is trivial to show that these variational principles lead to the exact real time propagator and imaginary time propagator if we use the full Hilbert space. Once we solve the variational equations we can evaluate $\text{Tr} \rho(t)$ and perform a Fourier analysis in the case of real time to obtain the micro-canonical level density, or extract the free-energy in the case of imaginary time.

These are the basic ideas of the extension of the TDMD method to propagators. That is, we use variational principles for the propagators under the assumption that they are written as a sum of time dependent elementary propagators of the type $\exp(a^\dagger u a)$.

We note that our method is very different from functional integrals based on the Hubbard-Stratonovich transformation (ref.[2]). With functional integrals we end up with multidimensional integrals of propagators, and they are hardly computable with Monte Carlo methods. The same can be said for imaginary time functional integrals, although in some cases the partition function is amenable to Monte Carlo evaluation. Moreover, in the case of the partition function our method is very different from the minimization of the free energy functional (see
for example ref. [3]). In this latter method the free energy is a functional of a density operator (in some sense the propagator we have just described) which must be minimized to obtain the actual propagator. The major stumbling block of this method is that we do not know how to compute the entropy in presence of a projector to good quantum numbers or if the density operator is a sum of elementary propagators. This difficulty has been the major hurdle in using the temperature dependent Hartree-Fock, or Hartree-Fock-Bogoliubov methods in presence of exact projectors to good quantum numbers. This work deals mostly with formalism and only a few numerical examples.

The outline of this work is the following. In section 2 we derive in detail the equations of motion. In section 3 we discuss a few properties in the imaginary time case. In section 4 we discuss the equations of motion for the real time propagation, conservation laws, and how one can extract the micro-canonical level density from the Fourier transform of real time propagators. In section 5 we discuss a few numerical examples in a simplified Hilbert space.

2 The equations of motion.

As a notation, we use a caret to denote second quantized operators and we denote elementary propagators (EP) as

\[ \hat{U} = \exp[\sum_{ij} a_i^\dagger u_{ij} a_j] \]  

(10)

where the sum runs over the single-particle space \( i = 1, 2, ..., N_s \). The matrix \( u \) is time dependent. As well known, EP’s form a group (ref.[4]), and the product of
two EP’s is an EP. Also, to any EP we can associate the matrix (which we denote without the caret)

\[ U = \exp(u) \tag{11} \]

Throughout this work, small letters will denote the logarithm of matrices as in eq.(11) which are denoted with capital letters. In this work we do not consider the most general EP, where we allow for particle number violation as done in the Hartree-Fock-Bogoliubov formalism. The group property is still valid in such a case and it is the cornerstone of the method. Given two EP’s such as \( \hat{S} \) and \( \hat{T} \) represented by \( S \) and \( T \) respectively, the product \( \hat{T}\hat{S} \) is represented by \( TS \). Moreover, traces taken in the full Hilbert space will be denoted as \( \text{Tr} \) and traces taken in the single-particle space as \( \text{tr} \). Since we shall consider traces in the Hilbert space, we start with Grand-Canonical traces, and we consider since the beginning, projectors to good quantum numbers, which we write schematically as

\[ \hat{P} = \sum_E d^*(E)\hat{R}(E) \tag{12} \]

where \( \hat{R}(E) \) is a rotation operator (which is an EP) dependent on the three Euler angles, in the case of the angular momentum projector, or is the operator \( \exp(\alpha\hat{N}) \), \( \hat{N} \) being the particle number operator, in the case of particle number projector. In this latter case \( \alpha \) is a purely imaginary phase \( 2i\pi k/N_s \) with \( k = 1, 2, \ldots, N_s \). Similarly we can recast the parity projector as in eq.(12). The detailed form of \( d^*(E) \) can be found in many textbooks (see for instance ref.[5]). The ansatz for the propagator is

\[ \hat{\rho} = \sum_{D=1}^{N_D} \hat{S}_D \tag{13a} \]

and

\[ \hat{\rho}^\dagger = \sum_{D'=1}^{N_D} \hat{T}_{D'} \tag{13b} \]
we use this notation since often we omit the labels $D$ and $D'$, in order to shorten the equations, with the understanding that $\hat{T}_{D'} = \hat{S}_{D'}^\dagger$. Consider the following traces

$$\text{Tr}[\hat{\rho}^\dagger\hat{P}\hat{\rho}] = \sum_{D'} \sum_D \sum_E d^*(E) \text{Tr}[^S^T^R]$$

(14)

where, again, $\hat{T}$ is labeled by $D'$ and $\hat{S}$ by $D$. Note that we have used the cyclic property of the trace. Using the aforementioned group property and the identity

$$\text{Tr} \hat{W} = \det(1 + W)$$

(15)

valid for any EP, we have

$$\text{Tr}[\hat{\rho}^\dagger\hat{P}\dot{\hat{\rho}}] = \sum_{D'} \sum_D \sum_E d^*(E) \det[1 + STR]$$

(16)

To obtain the time derivative of $\dot{\hat{\rho}}$. Let us vary eq.(16) with respect to all $S$’s. Using the identity, valid for any matrix $M$,

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

(17)

we obtain

$$\text{Tr}[\hat{\rho}^\dagger\hat{P}\dot{\hat{\rho}}] = \sum_{D'} \sum_D \sum_E d^*(E) \det[1 + STR] \text{tr}(F \dot{STR})$$

(18)

where

$$F = (1 + STR)^{-1}$$

(19)

Next, we evaluate the variation of eq.(18) with respect to a specific $T_{aa'}D'$ where $a, a'$ are single-particle indices. Again using the identity of eq.(17) we obtain

$$\delta_{T_{D'}} \text{Tr}[\hat{\rho}^\dagger\hat{P}\dot{\hat{\rho}}] = \sum_D \sum_{E} d^*(E) \det[1 + STR] \times$$

$$\left[ \text{tr}(RFS\delta T) \text{tr}(RFST) - \text{tr}(RFSTRFS\delta T) + \text{tr}(RF\delta T) \right]$$

(20)
Hence
\[
\frac{\partial T_{aa'D'}}{\partial T_{aa'D'}} \text{Tr}[\dot{\rho}^\dagger \dot{\hat{\rho}}] = \sum_D \sum_E d^*(E) \det[1 + STR] \times \\
(\text{tr}(RF\dot{S}T)RFS - RF\dot{S}TRFS + RF\dot{S})_{a'a'D'}
\]  
(21)

We now have to evaluate the right hand side of the variational equations. Let us assume that we have lumped together the kinetic energy and the two-body potential, as normally done in the shell model, and that
\[
\dot{H} = \frac{1}{2} \sum_{ijkl} H_{ijkl} a_i^\dagger a_j^\dagger a_l a_k
\]  
(22)

where \(H\) is already antisymmetrized (i.e. \(H_{ijkl} = -H_{ijlk}\)). We have
\[
\text{Tr}(\dot{\rho}^\dagger \dot{\hat{H}}) = \sum_{D'\in D} \sum_E d^*(E) \det[1 + STR] \times [\text{tr}(\Gamma)N] + 2\text{tr}(RF\Gamma FS \delta T)]
\]  
(23)

where
\[
N = 1 - F
\]  
(24)

and (the sum over repeated indices is assumed)
\[
\Gamma_{kl} = H_{ikjl} N_{ji}
\]  
(25)

We have then
\[
\delta_{T_{aa'D'}} \text{Tr}(\dot{\rho}^\dagger \dot{\hat{H}}\dot{\rho}) = \sum_D \sum_E d^*(E) \det[1 + STR] \times \\
[\text{tr}(\Gamma N)\text{tr}(RFS\delta T) + 2\text{tr}(RF\Gamma FS \delta T)]
\]  
(26)

Hence for a specified \(T_{aa'D'}\) we have for the right hand side, which we call \(R\),
\[
R_{(1)a'a'D'} = \sum_D \sum_E d^*(E) \det[1 + STR] \times [\text{tr}(\Gamma N)(RF) + 2(RF\Gamma FS)_{a'a}]
\]  
(27)

We are now in a condition to write down explicitly the equations of motion. Let us consider first the imaginary time case. We have for \(\dot{S}\) (the superscript refers to EOM1),
\[
L_{(1)a'a'D',b,b'D',\dot{b},\dot{b}'D'} = -R_{a'a'D'}
\]  
(28)
The matrix $L$ can be read off from eq. (21) and is given by the following expression

$$L_{a' D', b', b D}^{(1)} = \sum_E d^*(E) \det[1 + STR] \times

[(RF S)_{a' a}(TRF)_{b' b} - (RF)_{a' b}(TRFS)_{b' a} + \delta_{b' a}(RF)_{a' b}]$$  (29)

In the case of real time propagation the equation of motion EOM1 is

$$L_{a' D', b', b D}^{(1)} \dot{\psi}_{bb'} = -i R_{a' a D}^{(1)}$$  (30)

The equations of motion EOM2 can be obtained in a similar way. We first evaluate $\text{Tr}[\dot{\hat{\rho}}\hat{\rho}]$ and then we vary the result with respect to $S_{aa' D}$. We simply write the result as

$$L_{a' a D', b', b D}^{(2)} \dot{\hat{T}}_{bb'} = i R_{a' a D}^{(2)}$$  (31)

for real time propagation and

$$L_{a' a D', b', b D}^{(2)} \dot{\hat{T}}_{bb'} = - R_{a' a D}^{(2)}$$  (32)

in the case of imaginary time. The matrices in eqs. (31) and (32) have the following expressions

$$L_{a' a D', b', b D}^{(2)} = \sum_E d^*(E) \det[1 + STR] \times

[(RF S)_{b' b}(TRF)_{a' a} - (RF)_{b' a}(TRFS)_{b' b} + \delta_{b' b}(RF)_{a' a}]$$  (33)

and

$$R_{a' a D}^{(2)} = \sum_{D'} \sum_{E} d^*(E) \det[1 + STR][\text{tr}(\Gamma) \hat{N}(TRF) + 2(TRFTF)]_{a' a}$$  (34)

In the case of real time EOM1 and EOM2 are the complex conjugate of each other.

If we consider neutrons and protons separately we simply have to add the extra isospin index to the single-particle indices. In such a case it is convenient to choose the matrices $S$ as block diagonal, i.e. the matrix $S$ does not couple
neutrons and protons. This choice makes the projection to the proper number of neutrons and protons easier.

3 Some properties of the propagators for imaginary time.

Let us consider the imaginary time equations of motion. Let us assume that at some initial time $t_0$ the propagator is a sum of hermitian EP’s and a sum of non-hermitian EP’s plus their hermitian conjugates. We then can say that for each $\hat{S}_D$ there is a $T$ (which can be $D$ itself) such that $S^\dagger_{aa'D} = S_{aa'D}$, or $S^*_{a'aD} = S_{aa'D} = T_{a'a'D}$. Let us prove that the time evolution preserves the hermitian structure of $\hat{\rho}$ and that EOM2 is equivalent to EOM1. These two properties are essential from a physical point of view. In order to do so, let us set

$$\mathcal{O} = \text{Tr}(\hat{\rho}^\dagger \hat{P} \hat{\rho})$$
$$\mathcal{E} = \text{Tr}(\hat{\rho}^\dagger \hat{H} \hat{\rho})$$

(35)

Since the projector satisfies the relations $\hat{P}^\dagger = \hat{P}$ and $\hat{P}^2 = \hat{P}$ the above functional are real. Moreover we can rewrite EOM1 schematically as (using the sum convention)

$$\frac{\partial^2 \mathcal{O}}{\partial T_{a'a'D} \partial S_{b'b'D'}} \dot{S}_{b'b'D'} = - \frac{\partial \mathcal{E}}{\partial T_{a'a'D}}$$

(36)

which can be rewritten as

$$\frac{\partial^2 \mathcal{O}}{\partial S_{a'aD} \partial S_{b'b'D'}} \dot{S}_{b'b'D'} = - \frac{\partial \mathcal{E}}{\partial S_{a'aD}}$$

(37)

Taking the complex conjugate of eq. (37) we have

$$\frac{\partial^2 \mathcal{O}}{\partial S_{a'aD} \partial S_{b'b'D'}} (\dot{S}_{b'b'D'})^* = - \frac{\partial \mathcal{E}}{\partial S_{a'aD}}$$

(38)
Hence, comparing eqs. (37) and (38) we have

\[(\dot{S}_{bb'}^{D'})^* = \dot{S}_{vb}^{D'}\]  \hspace{1cm} (39)

that is \(\dot{S}_{D'} = \dot{S}_{D'}^\dagger\). This implies that

\[(S + dt\dot{S})^D_D = (S + dt\dot{S})^D_D\]  \hspace{1cm} (40)

Strictly this is true if the solution of the system of eq.(37) is unique. If we have multipole solutions we can always force eq.(38) and still satisfy eq.(37). This property guarantees that the spectrum of \(\hat{\rho}\) is real.

Next, EOM2 can be rewritten as

\[\partial^2 O / \partial S_{aa'} D \partial T_{bb'} D' \hat{T}_{bb'} D' = - \partial E / \partial S_{aa'} D\]  \hspace{1cm} (41)

which can be recast as

\[\partial^2 O / \partial S_{aa'} D \partial S_{bb'} D' \hat{T}_{bb'} D' = - \partial E / \partial S_{aa'} D\]  \hspace{1cm} (42)

which implies that \(\hat{T}_{bb'} D' = \hat{T}_{bb'} D'\). Therefore EOM2 gives the same solution as EOM1.

4 The propagators for real time.

3a. Micro-canonical level density and constants of motion.

The equations discussed in the previous section are not easy to solve. In fact, we expect that the numerical solution will show an exponential behavior as a function of the imaginary time and therefore some kind of numerical stabilization
might be necessary especially for large values of imaginary time. In this section we discuss the real time propagation and a motivation on physical grounds.

Let us assume that we have solved EOM1 (or EOM2) as a function of the time and let us evaluate

$$f(t) = \text{Tr} \hat{\rho}(t) \quad (43)$$

Consider the following Fourier transform

$$g(\omega) = \frac{1}{\pi} \text{Re} \int_0^\infty dt f(t) e^{i(\omega+i\gamma)t} \quad (44)$$

in the limit of $\gamma \to 0^+$. The function $g(\omega)$ approaches the level density if we have evaluated $f(t)$ with sufficient accuracy for the Hamiltonian $\hat{H}$. There are a number of points to be discussed. Consider first some conservation laws which must be satisfied if we have solved the equations of motion accurately. We shall prove that the quantities defined in eq.(35) are constants in time. Let us rewrite EOM1 and EOM2 in the following form

$$\frac{\partial^2 \mathcal{O}}{\partial S_{aa'}^{*} D \partial S_{bb'}^{*} D'} \dot{S}_{bb'}^{D' D} = -i \frac{\partial \mathcal{E}}{\partial S_{aa'}^{*} D} \quad (45)$$

and

$$\frac{\partial^2 \mathcal{O}}{\partial S_{aa'}^{*} D \partial S_{bb'}^{*} D'} \dot{S}_{aa'}^{D' D} = i \frac{\partial \mathcal{E}}{\partial S_{aa'}^{*} D} \quad (46)$$

Multiplying eq.(45) by $\dot{S}_{bb'}^{D' D}$ and summing over the indices, multiplying eq.(46) by $\dot{S}_{aa'}^{D' D}$ and summing over the indices, and subtracting the two results one has

$$\frac{\partial \mathcal{E}}{\partial S_{aa'}^{*} D} \dot{S}_{bb'}^{D' D} + \frac{\partial \mathcal{E}}{\partial S_{aa'}^{*} D} \dot{S}_{aa'}^{D' D} = 0 \quad (47)$$

The above is the time derivative of $\mathcal{E}$.

The conservation of $\mathcal{O}$ is slightly more involved to prove. Consider EOM1 as given by eq.(30) and EOM2 given by eq.(31). Let us multiply EOM1 by $T_{aa'}^{D'}$
and sum over the indices, and EOM2 by $S_{aa'D}$ and sum over the indices and add the two results. We obtain, using the cyclic property of the trace and the definitions of $F$ and $N$

$$\frac{d}{dt} \sum_E d^*(E) \sum_{DD'} [\text{det}(1 + S TR) \text{tr}(N)] = 0$$

(48)

Let us now consider separately the particle number projection from the rest of the projectors to good quantum numbers, in the following way. Let us define the complex fugacity $z = \exp(\alpha)$ and isolate it from the rest of the rotation operator. Then

$$\frac{d}{dt} \sum_E d^*(E) \sum_{DD'} [\text{det}(1 + z S TR) \text{tr}(N)] = 0$$

(49)

and

$$N = z S TR/(1 + z S TR)$$

(50)

The exact projection to the proper number of particles $A$ can be done by isolating the coefficient of $z^A$ in $\text{det}(1 + z S TR) \text{tr}(N)$. Let us consider the diagonal representation of the matrix $W = S TR$ and let us call $\omega_\mu$ its eigenvalues. Recall (although we work in real time) that $\text{det}(1 + z S TR)$ is a grand-canonical partition function and that the canonical partition function for $A$ particles is given by

$$C(A) = \sum_{\mu_1 < \mu_2 < ... < \mu_A} \omega_{\mu_1} \omega_{\mu_2} ... \omega_{\mu_A}$$

(51)

This is a homogeneous polynomial of power $A$ in the $\omega$’s for which the Euler’s theorem holds. Let us call $C(A-1, \mu)$ the canonical partition function for $A-1$ particles with the level $\omega_\mu$ removed. Then eq. (49) can be rewritten as

$$\frac{d}{dt} \sum_E d^*(E) \sum_{DD'} \sum_\mu \omega_\mu C(A-1, \mu) = 0$$

(52)

Since $C(A-1, \mu) = \partial C(A)/\partial \omega_\mu$ the Euler’s theorem gives $\sum_\mu \omega_\mu C(A-1, \mu) = AC(A)$, and therefore

$$\frac{d}{dt} \sum_E d^*(E) \sum_{DD'} C(A) = 0$$

(53)
hence the particle-number projected overlap is a constant of motion. These two
conservation laws are a valuable test in order to control the accuracy of the time
evolution. There are a few remaining points which will discussed in the next
subsection.

3b. The choice of the initial conditions.

We have described in detail the form of the equations of motion but so far we
have not specified the initial condition at $t = 0$. Ideally we would set $\rho = 1$. This
choice is necessary if we wish to evaluate the micro-canonical level density using
eq(44). Note however that we are solving an initial value problem and in principle
we can take any initial $\rho(0)$. If we consider $\rho(0) = 1$, we can only consider one
single EP. There is simply no way to have $\rho(0) = 1$ with several independent EP’s.
In the case of several EP’s we have several choices. Consider for a moment the
decomposition of the Hamiltonian $\hat{H}$ into a sum of quadratic operators of the type

$$\hat{H} = \hat{h} - \sum \hat{Q}^2$$

much is the same way it is done as a preliminary step to express the propagator with functional integrals. In eq.(54) $\hat{h}$ and $\hat{Q}$ are one body operators. The
propagator after a small time interval $\delta t$, up to $\delta t^2$ terms, can be be written as

$$\rho(\delta t) = \exp(-i\delta t\hat{h}) + 1/2 \sum [\exp(i\sqrt{\delta t}\hat{Q}) + \exp(-i\sqrt{\delta t}\hat{Q})]$$

As an initial start we can consider few terms of this type. In practice we do the
following instead. Consider simply a sum of the type

$$\rho(\delta t) = \sum \exp(-i\delta t\hat{s})$$

where $\hat{s}$ are one body operators, unspecified for the moment. For sufficiently
small $\delta t$, only their sum contributes to the propagator, that is, the ansatz of eq.(56)
is equivalent to the choice of just one EP. Hence we first start from \( \rho(0) = 1 \), using only one EP. We solve up to \( \delta t \) the equations of motion and we decompose \( S(\delta t) \) into a sum of different EP’s. Such a sum of independent \( S_D \) is our choice for the initial start. The set of \( S_D \) is then evolved up to finite times. Since the decomposition of the initial \( S \) (for \( N_D = 1 \)) into several \( S \)’s is arbitrary, we expect the solution of the equations of motion is not unique. That is the matrix \( L \) can have 0 eigenvalues. We test the eigenvalues of \( L \) and we solve the linear system of equation (45) in the unknowns \( \hat{S}_{bb'}D' \) in the basis that diagonalizes \( L \). In doing so, we discard all 0 eigenvalues and reconstruct \( \hat{S}_{bb'}D' \) in the original basis. That is we use the generalized inverse of \( L \). As a consistency test we verify that the \( \hat{S}_{bb'}D' \) obtained in this way satisfy the original system of eq.(45). An additional choice is to write \( \rho(0) \) as a sum of EP’s such that for small \( \delta t \rho(0) \) is proportional to 1 up to \( \delta t^2 \) terms. Note that in general especially for large single-particle spaces, the sizes of the linear system to be solved for \( \hat{S}_{bb'}D' \) can be very large and mathematical libraries such as SCALAPACK (ref.[6]) that can distribute large matrices into several processors are necessary. The time evolution of \( \rho \) is obtained using Runge-Kutta methods of high accuracy. We give a few examples of the numerical solution of the equations of motion in the next section. As a final remark, we found that even if our initial start for \( \rho \) is unitary, unitarity is broken as we evolve at finite times. This raises the question whether the number of levels obtained from eq.(44) is the correct one. We do not have in a strong argument regarding this point. However we can state that the integral over the energy of the micro-canonical level density has the correct value. The argument is the following. Consider first the case of one EP. The projected overlap at \( t = 0 \) is simply the projected trace of the unity operator. Hence it is simply the total number of levels. Such an overlap
is a constant of motion, even if unitarity is broken at finite times. In the case of several EP’s, since at the initial time we decompose the propagator obtained after a small time interval $\delta t$ into several EP’s, the energy integrated micro-canonical level density is the same (up to $\delta t^2$ terms) and, again, after we solve the equations of motion at finite time, we obtain approximately the correct value.

5 A numerical example.

Let us consider a system of 6 neutrons in the $1s1p$ harmonic oscillator shells. We choose the harmonic oscillator frequency $\hbar \Omega = 12\, MeV$. For the interaction we take the neutron-neutron part of the N3LO interaction (ref.[7]) renormalized to the above single-particle space. This model is highly schematic and it serves solely to the purpose of testing the numerical method and the concepts of the previous sections. Since we solve the equations of motion in real time we must ensure to have the proper number of particles. We cannot use chemical potentials as usually done in the case of the imaginary time propagation. We also implement an angular momentum projector to $J_z = 0$. In one case we use the full angular momentum projector to $J = 0$. This model has only 10 states with $J_z = 0$ and 4 states with $J = 0$. The full space contains 28 states. In all calculations we take $\delta t$ in the range of $10^{-4} \div 10^{-5}$. Let us consider first one elementary propagator, that is $N_D = 1$. We start from $\rho(0) = 1$.

In fig.1 we show the error in the conservation of the energy-like quantity $\mathcal{E}(t)$ defined in eq.(35). Throughout this work we use $\hbar = 1$, that is, we measure the time in units of $MeV^{-1}$. In fig.2 we show the deviation from unitarity. As it
Figure 1: Variation $|\mathcal{E}(t)/\mathcal{E}(0) - 1|$ as a function of time.
can be seen, although the propagator is not unitary, $\mathcal{E}(t)$ is constant for very long times. In fig. 3 we show the micro-canonical level density given by eq. (44) as a function of the energy, together with the number function 

$$n(E) = \int_{\infty}^{E} dE' f(E')$$

(57)

The number function counts the levels from $-\infty$ up to a given energy $E$. We took in eq.(44) $\gamma = 0.1MeV$. In the limit $\gamma \rightarrow 0$, $f(E)$ is a sum of Dirac-delta functions and the number function increases by one unit anytime we cross a level. As it can be seen from fig.3, in some cases $n(E)$ increases by two units, which points out to a degeneracy (or near degeneracy) of two levels, not separated by $\gamma = 0.1MeV$. as a check, note that the total number of levels is the correct one.

In fig.4 we show the level density and the number function for $N_D = 1$ using
Figure 3: Level density $f(E)$ and number function $n(E)$ for $J_z = 0$. 
the full projector to $J = 0$. Note that the projector gives a different approximation to the full propagator compared to the $J_z = 0$ case.

Although very schematic and simple, these two examples show the main features of the formalism and properties described in the previous sections.

In conclusion, we have generalized the time dependent multi-determinant approach to propagators using variational principles of Dirac-type. We described in detail the equations of motion and showed that there are constants of motion not related to the unitarity of the propagator. Such constants of motion are very useful to test the correctness and accuracy of the numerical methods. In the future we plan to extend these numerical techniques to the neutron-proton case for reasonably large shell model spaces.
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