BEYOND TDHF : SCHRÖDINGER TIME-EVOLUTION IN A TRUNCATED SUBSPACE

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Abstract: We derive non-determinantal approximations to the Schrödinger time-evolution in a necessarily truncated subspace, that allow for a flux of probability between the subspace and the excluded space. A second-order time-differential equation in the subspace and a time-dependent optical potential are studied in a number of examples.

1. INTRODUCTION

Going beyond the Time-Dependent Hartree Fock approximation will generally require a big step backward in the dimensionality of the space within which the time evolution can be treated. While the time-evolution of a TDHF determinant is generally not confined to a predetermined subspace of the total Hilbert space, non-determinantal approximations to the time-dependent Schrödinger solution will necessarily be restricted to a finite basis of small enough dimension to make the computation feasible. The truncation of the Hilbert space of the system to a small finite subspace leads to the problem of the coupling between the selected subspace and the excluded space, and how to account for the corresponding flux of probability between the spaces.

In the present paper we study non-unitary approximation methods that allow for a flux of probability but are completely defined and solvable within the subspace, such that the computation requires no information about the neglected space. The approximations are related[1,2] to a series expansion of the true subspace projection of the Schrödinger time-evolution operator, augmented in some cases by an "optical" time-dependent imaginary potential.

2. TRUNCATION OF THE SCHRÖDINGER PROBLEM

In stationary quantum mechanics many approximation methods consist in truncating the Hilbert space of the system to a limited subspace, and then solving the truncated problem in the subspace rather than dealing with the original Hamiltonian in the full space. A similar truncation procedure, when applied to the time-dependent Schrödinger equation, however, leads to unphysical results because the solution of the truncated problem is unitary with respect to the truncated subspace, and does not allow for any flux of probability between the selected subspace and the rest of the Hilbert space. Therefore the solution of the ordinary time-dependent Schrödinger equation in a truncated subspace artificially conserves all the initial probability (and mass, charge, energy etc.) within the subspace for all times, and thus differs qualitatively from the non-unitary subspace part of the true Schrödinger time-evolution. In general this property is the more undesirable the higher the truncation because the subspace probability will remain constant irregardless of how small the selected subspace is. For instance, the extreme truncation of the time-dependent Schrödinger-equation to dimension 1 would always lead to no time evolution at all (apart from a phase) whereas the true Schrödinger solution will in general immediately generate flux into states other than the initial state.

3. SECOND-ORDER SUBSPACE TIME-EVOLUTION EQUATION

We consider a Hilbert space that is devided into two orthogonal subspaces with corresponding projection operators P and Q,

$$P^2 = P,\ Q^2 = Q,\ P + Q = 1,\ PQ = 0 = QP \tag{1}$$

where P denotes the selected subspace and Q the excluded space.

In order to obtain an approximation to the time evolution in the subspace we rewrite the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\ \psi(t) = H\ \psi(t) \tag{2}$$

as a second-order equation

$$(i\hbar \frac{\partial}{\partial t})^2\ \psi(t) = H^2\ \psi(t), \tag{3}$$

project onto the P-space and insert $P^2 + Q^2 = 1$,

$$P\,H^2\psi = P\,H^2(P^2 + Q^2)\psi = (P\,H^2P)P\psi + (P\,H^2Q)Q\psi\,. \tag{4}$$

This yields for the P-space

$$-\hbar^2 \frac{\partial^2}{\partial t^2}\,\psi_P(t) = (H^2)_{PP}\,\psi_P + (H^2)_{PQ}\,\psi_Q \tag{5}$$

where the notation in analogy to Feshbach's optical model[3] has been used,

$$(H^2)_{PQ} = P\,H^2Q, \quad \psi_P = P\psi \quad \text{etc.} \tag{6}$$

Equation (5) describes the *exact* time evolution in the P-space for a given initial state and an initial time derivative as specified by eq. (2). The approximation consists in neglecting the $\psi_Q(t)$ term in eq. (5). In practical cases the P-space will always be selected such that it contains the initial state, $\psi_Q(0) = 0$. Therefore the $\psi_Q(t)$ term will vanish during the first time step and it should be reasonable to neglect it for sufficiently small intervals of time. This yields the second-order subspace time-evolution equation

$$-\hbar^2 \frac{\partial^2}{\partial t^2}\,\psi_P(t) = (H^2)_{PP}\,\psi_P(t) \tag{7a}$$

with the initial conditions

$$\psi(t=0) = \psi_P(t=0), \quad \psi_Q(t=0) = 0 \tag{7b}$$

and

$$i\hbar \frac{\partial}{\partial t}\,\psi_P(t) = H_{PP}\,\psi_P(t) \qquad (t=0). \tag{7c}$$

In general H_{PP} and $(H^2)_{PP}$ do not commute, and the approximate subspace time-evolution (7) is *non-unitary* as desired. In particular the exact flux of probability between the P- and Q-space is approximated rather accurately in many cases. This will be demonstrated below in a number of examples.

We note that a second (or higher order) equation is essential for a non-unitary solution. The ordinary time-dependent Schrödinger equation (2), when truncated in the same way as eq. (5) leads to the truncated Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\,\psi_P(t) = H_{PP}\,\psi_P(t) \tag{8}$$

with the undesirable unitary solutions.

4. SOLUTION OF THE SUBSPACE TIME-EVOLUTION EQUATION

Although the second-order subspace time-evolution equation (7) allows for a flux of probability out of the subspace (and back), it is completely defined within the subspace. In particular, the matrix elements of $(H^2)_{PP}$ can be computed in any P-space basis without information about the neglected Q-space. Equation (7) can easily be solved in the P-space representation that makes $(H^2)_{PP}$ diagonal. Thus the solution of eq. (7) requires one matrix diagonalization for all times, a numerical effort that does not exceed the one necessary for solving the (inappropriate) truncated Schrödinger equation (8).

For short time intervals an expansion to second order in time with the first and second derivative specified by eq. (7) is superior to diagonalizing $(H^2)_{PP}$,

$$\psi_P(t) = [1 - i H_{PP} t/\hbar - (H^2)_{PP} t^2/2\hbar^2]\psi_P (t=0) + \mathcal{O}(t^3). \qquad (9)$$

Such an expansion for short time steps may be important, e.g. for describing the first contact in a heavy-ion collision, or for an explicitely time-dependent Hamiltonian (e.g. in a semiclassical collision study with the center-of-mass motion given along some path).

5. EXAMPLES

5.1 Lipkin model

As a first example we consider the Lipkin model[4-7], a popular test case for time-dependent approximations to the exact Schrödinger solution. The model describes an exactly solvable many-body system consisting of N fermions on two N-fold degenerate levels evolving in time under the Hamiltonian

$$H = \frac{\varepsilon}{2} \sum_{p\sigma} \sigma a^+_{p\sigma} a_{p\sigma} + \frac{V}{2} \sum_{pp'\sigma} a^+_{p\sigma} a^+_{p'\sigma} a_{p'-\sigma} a_{p-\sigma} \qquad (10)$$

with the creation and anihilation operators of the single particle states $|p,\sigma\rangle$ where $p = 1,\ldots,N$ labels the degenerate states of both levels $\sigma = \pm 1$.

In the example of fig. 1 the system consists of 8 particles. The full Hilbert space of the system has dimension 9 and the subspace is truncated to dimension 5 ($|JM\rangle = |J-J\rangle,\ldots,|JO\rangle$ in the standard basis).

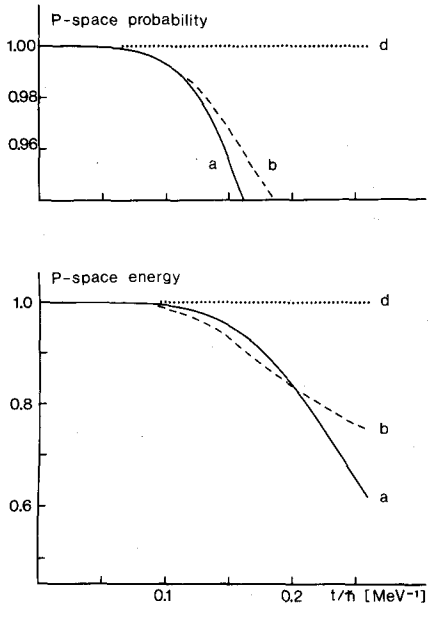

Fig. 1: Eight-particle Lipkin model (dimension 9) truncated to dimension 5.

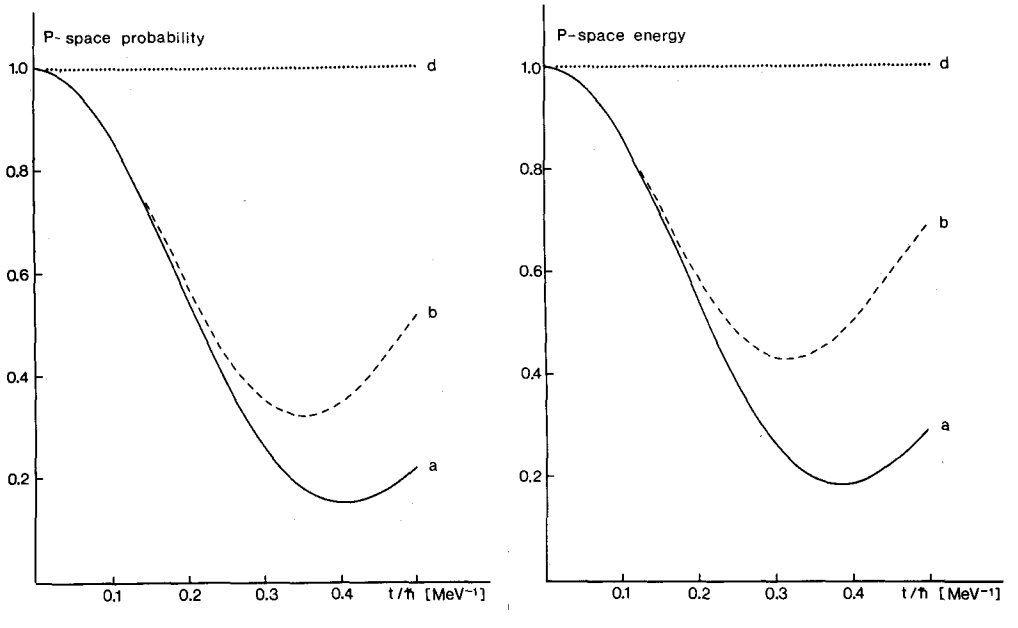

Fig. 2: Gaussian 100 x 100 Hamiltonian truncated to 10 x 10.

The initial state has M=-J and the parameter set is ε=1, V=1. The figure shows the loss of probability and the loss of energy out of the subspace as a function of time for both the exact Schrödinger time evolution (a) and the subspace approximation (b) of eq. (7). The approximation (b) remains rather accurate over a time interval during which a sizable flux of probability and energy out of the subspace occurs. This is much superior to the truncated Schrödinger calculation (d) of eq. (8) which results in no loss of probability and energy for all times. Other examples with different parameter sets and different initial conditions lead to qualitatively similar results.

5.2 Gaussian matrix parametrization

We have studied[2] the behaviour of the subspace time evolution approximations for a number of schematic Hamiltonian matrices with exponential diagonal level density and a Gaussian fall-off for the off-diagonal matrix elements with or without random signs. This parametrization comprises constant and diagonal Hamiltonians, C-numbers and intermediate cases.

In the example plotted in fig. 2a the exact solution for a 100 x 100 Hamiltonian matrix is compared with the P-space approximation (7) for the first 10 x 10 components for an initial state peaked at the second and third basis state in the P-space. Here the probability in the P-space, as described by the non-linear approximation (b), is remarkably close to the exact result (a), even though a substantial flux of probability out of the P-space occurs. For instance, after a loss of 30% of the initial P-space probability the non-linear subspace approximation (7) remains within 1% of the exact result. This is clearly superior to the truncated result (d) which (arbitrarily) conserves the P-space probability. Although the non-linear approximation becomes less accurate for longer time intervals it still reproduces the qualitative behaviour of the exact solution. In particular a flux back from the neglected space into the P-space occurs almost simultaneously in the exact (a) and approximate (b) result.

The flux of probability between P- and Q-space is associated with a similar flux of energy, that is shown in fig. 2b. Here again the non-linear subspace approximation (b) is much superior to the truncated result (d). It is rather accurate over a sizable interval of time (e.g. 3% at an energy loss of 30%). Other cases are discussed in ref.2.

5.3 Exactly solvable Hamiltonians

For any Hamiltonian with the property

$$(H^2)_{PQ} = 0 = (H^2)_{QP} \tag{11}$$

the subspace approximation (7) leads to an *exact* solution in the P-space. In order to demonstrate that this class of Hamiltonian matrices comprises cases with substantial flux of probability between the spaces we consider the particularly simple example

$$(H_{PP})_{mn} = -\sqrt{\exp\ (-\alpha n)}\quad \delta_{mn} = -(H_{QQ})_{mn}, \tag{12}$$

$$(H_{PQ})_{mn} = \gamma\ \delta_{mn} = (H_{QP})_{mn}. \tag{13}$$

Here the P-space probability can be given analytically as a function of time. The result for one set of parameters (α,γ) and different initial states β is given in figure 3. It shows that the probability tends to oscillate in time between the P- and Q-space. The Q-space probability can be quite large (even though the spaces are disconnected with respect to the second order equations and $\psi_Q(0) = 0$). Since in the case we have considered, the second-order approximation is *exact*, it is very much better than the usual truncation procedure (which would arbitrarily conserve the subspace probability and energy for all times).

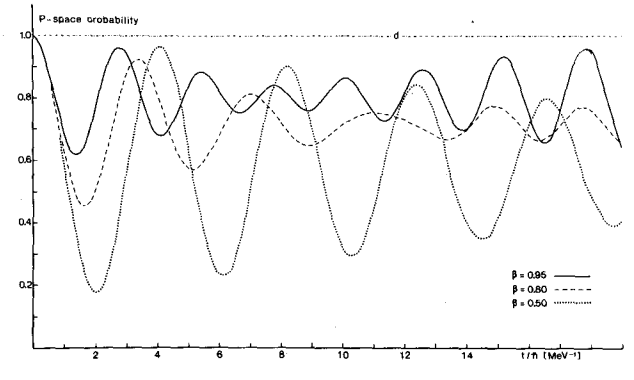

Figure 3: Coincidence of exact and approximate solution in the case $(H^2)_{PQ} = 0$, for different initial distributions β, and a 50% truncation to dimension 11. Curve d is the solution of the Schrödinger equation in the subspace.

6. PROJECTION OF THE TIME-EVOLUTION OPERATOR

An explanation why the approximation (7) is in many cases rather close to the exact time evolution in the subspace can be given in terms of the time-evolution operator

$$U(t) = \exp(-i\,H\,t/\hbar) = \sum_{n=0}^{\infty} (-i\,t/\hbar)^n/n!H^n. \qquad (14)$$

The application of the projection and insertion of $P^2 + Q^2$, similar to eq. (4), yields

$$\psi_P(t) = \sum_{n=0}^{\infty} (-i\,t/\hbar)^n/n!\ (H^n)_{PP}\ \psi_P(0) \qquad (15)$$

for an initial state $\psi(0) = \psi_P(0)$ in the P-space. This is the exact P-space time evolution for all times. Up to second order in time the expansion (15) is identical to the approximation (9) of sect. 3. Thus this approximation can be viewed as a first step away from the unitary solution of the truncated Schrödinger equation (8) towards the exact non-unitary solution (15) for the first time step. It turns out that, in many cases, the inclusion of the H^2 term alone already leads to a rather accurate approximation of the flux of probability into the Q-space.

7. TIME DEPENDENT "OPTICAL" POTENTIAL

The success and wide-spread use of the optical model to correct for the excluded channels in stationary scattering theory has motivated us to study if a similar, but time dependent, "optical" potential[7] can be used to account for the flux of probability out of the truncated subspace in a time-dependent calculation.

The problem consists in adding to the truncated Hamiltonian an appropriate imaginary time-dependent matrix i W(t) such that the "optical" solution $|\phi\rangle$ of the modified subspace Schrödinger equation

$$i\,\hbar\,\frac{\partial}{\partial t}\,|\phi\ (t)\rangle = [H_{PP} + i\,W(t)]\ |\phi\rangle \qquad (16)$$

fits the subspace part of the exact solution $|\psi(t)\rangle$ as closely as possible

$$|\phi(t)\rangle \approx P\ |\psi(t)\rangle\ . \qquad (17)$$

Figure 4 shows an example of such an optical potential fit for a schematic heavy-ion model. Here the Hamiltonian

$$H = H_{sp}^{(1)} + H_{sp}^{(2)} + V(1,2) \qquad (18)$$

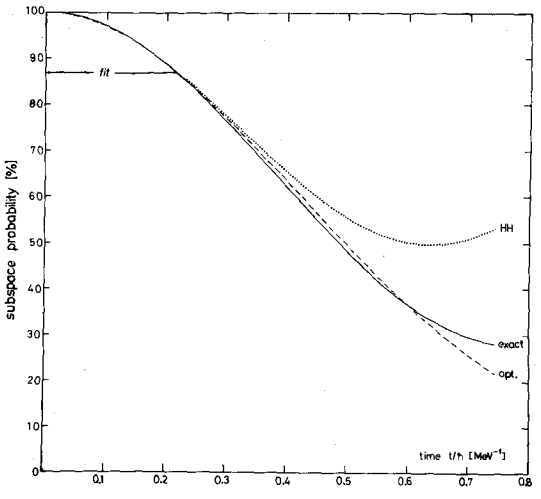

Figure 4: Optical potential fit for a schematic time-dependent heavy-ion collision model.

consists of single-particle (sp) terms for each ion and a two-body interaction term. The single-particle energies are taken to have a level-density form

$$H_{sp}^{(1)} \; |i\rangle = V_1 \exp(-i/a_1)\,|i\rangle \tag{18a}$$

and

$$H_{sp}^{(2)} \; |j\rangle = V_2 \exp(-j/a_2)\,|j\rangle \quad , \tag{18b}$$

and the interaction matrix is defined in the product basis $|i\rangle\,|j\rangle$ as

$$\langle ij|V|kl\rangle = V_o \exp\{-(|ij-kl|\,/a_o^2)\} \tag{19}$$

with the parameters V_o, V_1, V_2 and a_o, a_1, a_2. The interaction is chosen such that the matrix elements should be large between two ion states $|i\rangle|j\rangle$ and $|k\rangle|l\rangle$ that are either particularly simple (e.g. low excited) or both very complicated (e.g. highly excited), and small for combinations of simple and complicated states.

We have studied a number of different functional forms for the optical potential iW that may lead to a satisfactory description of the time-evolution of the system. It turns out that a rather simple parametrization is already sufficient in many cases: The matrix iW can be chosen diagonal in the subspace "energy" representation

$$H_{PP}|n\rangle = \varepsilon_n|n\rangle \qquad (|n\rangle \in \text{P space}) \tag{20}$$

and linear in time, i.e.

$$\langle n' | iW | n \rangle = -i\bar{n} \, (\alpha_n + \beta_n \, t) \delta_{n'n} \quad , \tag{21}$$

where α_n and β_n are the fit parameters of the optical potential.

In the example plotted for a statistical initial distribution the full space of dimension 36 (i.e., 6 levels in each ion) is truncated to dimension 16 (i.e. the first 4 levels in each ion). During the time interval of fig. 4 the probability in the subspace decreases from initially 100% to about 30% before a flux of probability back into the selected subspace sets in. The optical approximation is fitted for the initial time interval $t \lesssim 1.4 \cdot 10^{-22}$ sec during which about 13% of the subspace probability is lost. Although the further loss of probability is quite large, the optical approximation remains close to the exact solution until the flux of probability back into the selected subspace starts to dominate. The latter effect is, of course, outside the scope of an optical model. Thus the extrapolation achieved by the optical model remains rather accurate over three times the period of time of the initial fit, and for more than five times the loss of probability within the original fit interval.

For simplicity the initial optical fit in fig. 4 has been made to the *exact* solution, which, of course, will not be known in practical cases. Therefore the optical model approach requires an initial time-evolution approximation which the optical potential can then be fitted to. The figure shows for comparison the second-order subspace approximation discussed in the previous sections (here labelled HH). It almost coincides with the exact solution within the fit interval of the optical potential but starts to deviate much earlier than the optical solution. It is therefore evident that the subspace approximation when combined with the optical model fit converges over a much larger interval of time.

8. SUMMARY AND CONCLUSIONS

The examples of the present paper show that the second-order subspace approximation, eq. (7), avoids the undesirable unitarity of the time-dependent Schrödinger solution within a truncated subspace that leads to an unphysical conservation of probability, mass charge and energy etc. within the selected subspace. The second-order time-differential equations (7) are completely defined and solvable within any given subspace, and the numerical effort required is comparable to that of

simply truncating the Schrödinger equation to the subspace. When expanded in powers of the Hamiltonian H (or time t) the second-order approximation coincides with the exact solution up to second order in H (and up to any order for certain classes of Hamiltonians). This may explain why the approximation is in many cases rather close to the exact result. In any case studied it turned out to be superior to the result of only truncating the time-dependent Schrödinger equation to the subspace (which approximates the exact time evolution only to first order in time).

We have also demonstrated that the approximation can be further improved by an appropriate time-dependent optical potential. According to our results, the optical model solution describes the flux of probability out of the selected subspace rather accurately but fails, as one would expect, when the flux back from the excluded space becomes important.

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