The time independent mean field method (TIMF) for the calculation of matrix elements of non relativistic propagators is based on a variational principle whose non linearity induces a multiplicity of variational solutions. Several of them can break any symmetry shared by the Hamiltonian and initial and final states. We describe a soluble model where, in particular, time reversal and parity breakings occur. Such breakings account for important properties of propagation amplitudes.

PACS numbers: 03.65.Nk, 24.10.-i, 34.10.+x

The observation of symmetry breakings in solutions of variational principles is familiar for static problems, such as those described by the Hartree-Fock method for deformed nuclei. Similar breakings can be expected for other variational theories, like the time independent mean field (TIMF) theory of reactions and decay. The TIMF method has already been implemented for various nuclear and atomic processes involving 3, 4, 5 and 8 particles and symmetry breakings were indeed found. In this letter we describe a soluble model which completely interpolates between mean field trial states and exact solutions. It provides a detailed observation of symmetry breakings as well as conservation. Because propagation amplitudes are obtained by saddle points rather than absolute maxima or minima, the multiplicity of solutions raises an ambiguity. The model shows that actually all mean field solutions should later be mixed linearly to recover, for the complete energy range, the best possible approximation of the exact solution.

We start from a Schwinger-like functional to calculate the amplitude $D(E) \equiv \langle \chi' | (E - H)^{-1} | \chi \rangle$ for propagation between initial and final states $\chi, \chi'$. The variation of $F$ gives, with appropriate normalizations,

$$
\begin{align*}
(E - H) | \Psi \rangle &= | \chi \rangle, \\
\langle \Psi' | (E - H) &= \langle \chi' |, \\
D(E) = \langle \chi' | \Psi \rangle &= \langle \Psi' | \chi \rangle,
\end{align*}
$$

with $(\Psi, \Psi')$ as a saddle point of $F$. For our model we consider a single-particle basis made of two square integrable orbitals $|a\rangle$ and $|b\rangle$, with single-particle energies $-1$ and $1$, respectively. In the resulting space for two distinct particles, spanned by $|a^2\rangle, |ab\rangle, |ba\rangle, |b^2\rangle$, we use for $H$ simply the corresponding sum of one-body Hamiltonians, with eigenvalues $-2, 0, 0$ and $2$, respectively. This is clearly a Hamiltonian invariant under particle exchange.
(denoted parity in the following) and complex conjugation (time reversal). Then we choose $|\chi'\rangle = |\chi\rangle$, and $\chi$ as a two-body state, described by a product of two identical, single-particle mixtures,

$$|\chi\rangle = (r|a\rangle + |b\rangle)_1 (r|a\rangle + |b\rangle)_2,$$

where $r$ is a frozen, real parameter. Both $\chi, \chi'$ are invariant under parity. The same holds for $\Psi, \Psi'$. Furthermore, since $|\chi\rangle = |\chi'\rangle$ and $r$ is real, time reversal symmetry is expressed by the property $|\Psi\rangle = |\Psi\rangle$ if $E$ is real, and $|\Psi\rangle = |\Psi\rangle$ if $E$ is complex, see Eqs.(2a,b).

It is seen trivially that the exact value of $D(E)$ is

$$D_{ex}(E) = \frac{r^4}{E+2} + \frac{2r^2}{E} + \frac{1}{E-2}. \tag{4}$$

This pole structure allows $E$ to remain real in the following. Our model investigates reconstructions of $D(E)$ with trial functions $\Psi, \Psi'$ restricted to less flexible forms,

$$|\Phi\rangle = c \quad a^2 > + s \quad a_1 b_2 > + t \quad b_1 a_2 > + st \quad b^2 >,$$

$$< \Phi | = c < a^2 | + u < a_1 b_2 | + v < b_1 a_2 | + uv < b^2 |. \tag{5}$$

where $c$ is a frozen, real parameter which expresses correlation constraints, and $s, t, u, v$ are four variational parameters, possibly complex. It is easily verified that, for the special value $c_{ex} = E^2/(E^2 - 4)$, the space of trial functions $\Phi, \Phi'$ contains the exact solutions $\Psi, \Psi'$ given by Eqs.(2), with $s = t = u = v = E/[r(E - 2)]$. Conversely, for $c = 1$, we generate a TIMF limit where the trial states $\Phi, \Phi'$ are uncorrelated, namely simple products of single-particle orbitals. The model thus achieves, as a function of $c$, an interpolation between a mean field approximation and an exact theory. Note that, despite its simplicity, the model is non trivial since the inverse of an additive one-body operator is a complicated sum of many-body operators. This letter studies whether time reversal, namely $s = u$ and $t = v$, on one hand, and on the other hand parity, namely $s = t$ and $u = v$, are properties conserved or broken by the variational principle.

With the restricted $\Phi, \Phi'$ of Eqs.(5), $F$ becomes

$$F = \frac{(cr^2 + rs + rt + st)(cr^2 + ru + rv + uv)}{E(c^2 + su + tv + stuv) - 2(stuv - c^2)}, \tag{6}$$

whose derivatives with respect to $s, t, u, v$ are easy to obtain. Let $F_s, F_t, F_u, F_v$ be the multivariate polynomial numerators of these derivatives. From the conditions $F_t = F_v = 0$ a straightforward, linear elimination of $t$ and $v$ in terms of rational functions of $s$ and $u$ is possible. The substitution of such rational fractions for $t$ and $v$ inside $F_s$ and $F_u$ then leaves two residual polynomial conditions for $s$ and $u$. It is finally easy, albeit slightly tedious, to eliminate for instance $u$ between these two polynomials and obtain a polynomial resultant $R(s; E, r, c)$, the roots of which designate the saddle points of $F$, Eq.(6).
It turns out that, except for spurious factors which either identically cancel \( F \) or make \( \Phi, \Phi' \) divergent, \( R \) reduces into the product of three simpler resolvents,

\[
\begin{align*}
R_{cc} &= c^2r(E + 2) + c(2c + cE - Er^2)s + (E + 2cr^2 - cEr^2)s^3 + r(2 - E)s^4, \\
R_{pb} &= cE(2c + cE + Er^2) + r(4c^2 + E^2 - c^2E^2)s + E(E - 2cr^2 + cEr^2)s^2, \\
R_{tb} &= cr(2c + cE + Er^2) + c(2r^4 - Er^4 + E + 2)s + r(2cr^2 - cEr^2 - E)s^2.
\end{align*}
\] (7a) (7b) (7c)

The first factor, \( R_{cc} \), generates four saddle points for which \( s = t = u = v \), namely both parity and time reversal are conserved. The second factor, \( R_{pb} \), induces two saddle points for which \( s = u \) and \( t = v \), but \( s \neq t \), hence parity is broken, while time reversal is conserved. The corresponding value \( F_{pb} \) of \( F \) is the same at both such saddle points,

\[
\frac{[r^2(c^2r^2 + c^2 + 2c - 1) + c^2]E^2 + 2c^2(1 - r^4)E - 4c^2r^2}{E(c^2E^2 - E^2 - 4c^2)}.
\] (8)

The last factor, \( R_{tb} \), induces two saddle points for which \( s = t \) and \( u = v \), but \( s \neq u \), hence parity conservation but time reversal breaking, with again equal values of \( F \) at both saddle points,

\[
F_{tb} = (c - 1) \frac{(cr^4 + 2r^2 + c)E + 2c(1 - r^4)}{(c^2 - 1)E^2 - 4c^2}.
\] (9)

While many combinations of the real parameters \( E, r, c \) induce real values for \( s, t, u, v \) at such symmetry breaking saddle points, see Figs.(1,2) for a \( pb^- \) and a \( tb \) saddle point, respectively, there are equally frequent situations where those pairs \( (s, t) \) or \( (s, u) \) which are not degenerate actually take complex conjugate values. Nevertheless, as shown by both Eqs.(8,9), the functional remains real valued. This allows useful analytic continuations of variational estimates of \( D \), which will indeed be plotted in several forthcoming Figures, regardless of the real or complex nature of the corresponding saddle points. Conversely, for the fully symmetric cases described by \( R_{cc} \), real estimates of \( D \) are obtained when \( s \) is real only, unless \( ReF \) is used as an estimate of \( D \) when \( F \) is complex.

By means of Fig.3 we now discuss the behaviors of the six estimates of \( D \) provided by \( R \) when \( c \) takes on all values between the limit without correlations, \( c = 1 \), and the limit allowing an exact result, \( c = c_{ex} \). We set \( r = -1.2 \) and \( E = 1.5 \) for Fig.3. Hence \( c_{ex} = -1.29 \) and \( D_{ex} = 0.51 \). The full lines show two branches of estimates provided by \( R_{cc} \). Its other two branches turn out to be either complex or out of range in that case. Not surprisingly, one of the full lines contains the point \((c_{ex}, D_{ex})\), representing the fully symmetric, exact solution \( \Psi, \Psi' \).

It is remarkable that the long-dashed line, which corresponds to the roots of \( R_{tb} \), also contains this exact point. It is also remarkable that the time reversal breaking, measured by \(|s - u|\) for instance, stays finite on that
long-dashed branch when \( c \) approaches \( c_{ex} \) and does not vanish at that point. It is nevertheless easy to verify that, when \( c = c_{ex} \), then \( F_{tb} \equiv D_{ex} \) as a function of \( E \) and \( r \). This indicates that, as long as correlations are allowed in the trial states, even partly only, the breaking of time reversal symmetry may help in finding good estimates of matrix elements of propagators. The paradox of a finite value of \( s - u \) at the exact point is understandable, because a well-known property of \( F \), see Eq.(1), is that only any one of the two equations, Eqs.(2), needs to be solved exactly to obtain \( D_{ex} \). It is unfortunate that, as shown by Eq.(9), the stationary value \( F_{tb} \) provided by uncorrelated trial states, namely for \( c = 1 \), identically vanishes.

The second full line branch goes through that same point \((c, D) = (1, 0)\). This is no accident, because \( R_{cc} \) gets a trivial, energy independent root \( s = -r \) when \( c = 1 \), for which the fully symmetric functional identically vanishes. Only three fully symmetric saddle points are left to depend on \( E \) for uncorrelated trial states, together with the \( pb \) branch. In the present case, besides that trivial fourth fully symmetric root \( s = -r = 1.2 \), one fully symmetric root is real and the other two are complex.

The short-dashed line on Fig.3 represents the behavior of the \( pb \) branch. It shows a vague trend to interpolate between the two real, fully symmetric branches, but its utility will be apparent later only. Indeed, it does not go through the exact point \((c_{ex}, D_{ex})\), nor does it show an accurate reproduction of \( D_{ex} \) for \( c = 1 \).

We show on Fig.4 the multivalued nature of the estimate(s) provided by the four roots of \( R_{cc} \). Obviously, the number of real roots depends on \( E, r, c \).

We now turn to behaviors of the estimates of \( D \) as functions of \( E \). This is illustrated by Fig.5, where \( D_{ex}(E) \) (full line) is compared to its various estimates with \( c = 1 \). It is seen at once that a fully symmetric estimate (dashed line) is convenient to reproduce pole behaviors near \( E = \pm 2 \). This is not completely surprising since the corresponding eigenstates \( |a^2> \) and \( |b^2> \) are themselves invariant under particle exchange. Conversely, eigenstates such as \( |a_1b_2> \) and \( |b_1a_2> \) are not invariant under such an exchange, and it is thus reasonable that a \( pb \) estimate is needed to account for the pole at \( E = 0 \). Moreover, it is consistent that the \( pb \) estimate fails for \( E \simeq \pm 2 \), and the fully symmetric estimate in turn fails for \( E \simeq 0 \). For the sake of completeness, we also show on Fig.5 the behavior of the \( tb \) estimate obtained when \( c = 0 \). It is clear that this \( tb \) estimate, like the \( pb \) one, succeeds for \( E \simeq 0 \) and fails for \( E \simeq \pm 2 \). All these properties are transparent from the corresponding special values of the functionals,

\[
F_{pb}|_{c=1} = \frac{(Er^2 + E + 2)(2r^2 - Er^2 - E)}{4E}, \quad (10a)
\]

\[
F_{tb}|_{c=0} = \frac{2r^2}{E}, \quad (10b)
\]

\[
F_{cc}|_{c=1} = \frac{(r + s)^4}{(s^2 + 1)(Es^2 - 2s^2 + E + 2)}, \quad (10c)
\]
The residues of the special values, Eqs.(10a,b), of $F_{pb}$ and $F_{tb}$ at $E = 0$ are $r^2$ and $2r^2$, respectively. This compares well with the exact residue $2r^2$, see Eq.(4). The three non trivial saddle points of $F_{cc}\left|_{c=1}\right.$ are the roots of

$$R_{cc}\left|_{c=1}\right. = r(2 - E)s^3 + Es^2 - Ers + (2 + E). \quad (11)$$

A straightforward elimination of $s$ between Eq.(11) and Eq.(10c) generates a cubic polynomial condition relating these three saddle point estimates $D_{cc}$ to $r$ and $E$,

$$16(4 - E^2)D_{cc}^3 + 8[12 + 6E - 2E^2 - E^3 + 6(E^2 - 4)Er^2 + (-12 + 6E + 2E^2 - E^3)r^4]D_{cc}^2 + \alpha D_{cc} + \beta = 0, \quad (12)$$

where $\alpha$ and $\beta$ depend on $r$ and $E$, naturally. For $E^2 = 4$ this polynomial, Eq.(12), reduces to degree 2 instead of 3, and the multivalued $D_{cc}$ has indeed first order poles for $E = 2$ and $E = -2$, with residues 1 and $r^4$, respectively. These agree with the exact residues, see Eq.(4).

Finally on Fig.6 we compare, for $r=1.1$, the exact $D$, as a function of $E$, with two kinds of estimates obtained with $c = 1$. The small-dashed line indicates the real root of Eq.(12), already found to show poles at $E = \pm 2$. The long-dashed line shows the real part of the other two roots of Eq.(12). Its complete lack of pole structure makes it much less valuable than the real root.

In conclusion, this letter gives three results for the variational theory of propagators. The first one is the existence of a non trivial and soluble model for mean field approximations, which are notoriously non linear and demand a sorting of their (intricate) solutions. The second result is indeed a complete classification of the solution branches of the model, with their physical meaning, namely symmetry conservation or breaking. We can keep track of their interconnection or lack of connection. We can also assess the validity domain of the amplitude estimate given by each branch. Of special interest are the time reversal breaking solutions which we discovered, because they can provide the exact amplitude and exist only if enough correlation is included in the trial states. When correlations are excluded, parity breaking solutions still exist and are absolutely necessary to account for several singularities of the exact amplitude. Fully symmetric solutions are not flexible enough, in the uncorrelated variational space, to account for all the singularities of the exact, fully symmetric solution, which is unique and correlated. The third result is then the necessity of a linear admixture of such solution branches, to remove any ambiguity of choices between them, patch their limited validity domains, and restore the uniqueness of the physical solution. As a first step for the representation of physical correlations, mean field solutions can thus be better analyzed along the lines described by this model.

Acknowledgements: A.W. thanks Service de Physique Théorique for its hospitality during part of the work.
[1] B.G. Giraud, M.A. Nagarajan and I.J. Thompson, Ann.Phys.(N.Y.) 152, 475 (1984).
[2] Y. Abe and B.G. Giraud, Nucl.Phys. A440, 311 (1985); J. Lemm, A. Weiguny and B.G. Giraud, Z.Phys. A336, 179 (1990); B.G. Giraud and M.A. Nagarajan, Ann.Phys.(N.Y.) 212, 260 (1991); B.G. Giraud, S.Kessal and L.C.Liu, Phys.Rev. C35, 1844 (1987); A. Wierling, B.G. Giraud, F.Mekideche, H.Horiuchi, T.Maruyama, A.Ohnishi, J.C.Lemm and A. Weiguny, Z.Phys. A348, 153 (1994).
[3] F. Mekideche and B.G. Giraud, J.Math.Phys. 34, 29 (1993); B.G. Giraud, Y. Hahn, F. Mekideche, and J. Pascale, Z.Phys. D27, 295 (1993).
[4] B.A. Lippmann and J. Schwinger, Phys.Rev. 79, 469 (1950); M. Gell-Mann and M.L. Goldberger, ibid. 91, 398 (1953); R. Balian and M. Vénéroni, Phys.Rev.Lett. 47, 1353 (1981).

FIG. 1. Contour plot of $F$, see Eq.(6), for $(s, t) = (u, v)$ when $(r, E, c) = (1, 3, -0.25)$. Vicinity of parity breaking saddle point $(s, t) = (-1.19, 0.13)$ with saddle value $F_{pb} = 0.46$.

FIG. 2. Contour plot of $F$ for $(r, E, c) = (1, 1, -0.25)$ and $(s, u) = (t, v)$. Vicinity of the time reversal breaking saddle point $(s, u) = (-0.73, -0.068)$ with saddle value $F_{tb} = 1.58$.

FIG. 3. Various estimates of amplitude $D$ as functions of the constraint $c$ for $(r, E) = (-1.2, 1.5)$. Full lines: full symmetry. Small-dashed line: parity breaking. Long-dashed line: time reversal breaking. Exact $D_{ex} = 0.51$ at $c_{ex} = -1.29$.

FIG. 4. Fully symmetric estimates as functions of $c$ for $(r, E) = (1, 1.5)$. Any folding of one of the full lines onto itself means a transition between two and four real estimates.

FIG. 5. Amplitudes as functions of $E$ for $r = -1.2$. Full line: $D_{ex}$. Dashed line: full symmetry estimate, $c = 1$. Short-dashed: $pb$, $c = 1$. Long-dashed: $tb$, $c = 0$. Poles demand full symmetry near $E = \pm 2$ and $pb$ or $tb$ near $E = 0$.

FIG. 6. Full symmetry estimates as functions of $E$ for $(r, c) = (1.1, 1)$. Short dashes: $F$ real. Long dashes: $ReF$, complex $F$. Full line: $D_{ex}$. Poles $E = \pm 2$ recovered by $F$ real.