Many-body dynamics on a time-dependent basis

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We propose a method of solution of the many-body Schrödinger equation that involves an expansion of the wave function in terms of a finite, time-dependent basis of a relevant subspace. The equations of motion for the expansion coefficients generalize previous proposals of approximate dynamics. The method is illustrated in the case of an N-particle system with an SU(2) Hamiltonian, and it is shown that it improves the approximation that disregards off-diagonal elements of the dynamical matrices.

I. INTRODUCTION

The dynamical many-body problem is a subject of current interest in view of the large field of applications to nuclear and molecular collisions as well as to quantum hydrodynamics. Among the most popular proposals to construct approximate solutions of the full Schrödinger equation, the time-dependent Hartree-Fock (TDHF) method is largely perferred, in spite of the fact that its validity is restricted to short times.[1] The traditional TDHF procedure[2] was enriched by the observation, posed by Lichtner and co-workers,[3] that the TDHF wave function should be endowed with a time-dependent phase proportional to the classical action computed on the TDHF path. On the other hand, Suzuki[4] introduces the action phases to establish his description of the semiclassical propagator that involves a superposition of Slater determinants (equivalently, coherent states) moving along independent TDHF trajectories. Being a semiclassical approximation of the exact propagator, the corresponding expression does not include interference terms.

In the present work we propose an alternative description of the dynamics, that, while preserving the quantal nature of the system, allows the introduction of trajectories on a classical phase space in the same spirit of Suzuki's propagator. For this sake, in Sec. II, we present the derivation of the law of motion of a wave function that is expanded on a set of predetermined moving states, starting from the Schrödinger equation. In Sec. III we discuss the particular realizations of our general dynamics, previously presented in the literature. An illustration that involves a two-level N-particle system with TDHF [SU(2)] coherent states as the moving set is presented in Sec. IV. Section V contains the final conclusions.

II. THE WAVE FUNCTION AND ITS EVOLUTION

Let us consider an instantaneous (not necessarily orthogonal) finite-dimensional basis $\{ | \varphi_i(t) \rangle \}$, where the dynamics of each member of the set is predetermined. A wave function

$$| \psi(t) \rangle = \sum_i a_i(t) | \varphi_i(t) \rangle \tag{2.1}$$

will be a solution of the Schrödinger equation provided that the time-dependent coefficients satisfy

$$i\hbar \sum_i \left[\dot{a}_i(t) - a_i(t) \left[\hat{H} - i\hbar \frac{\hat{\partial}}{\partial t} \right] \right] | \varphi_i(t) \rangle \equiv \sum_i \hat{v}_i | \varphi_i(t) \rangle = 0 . \tag{2.2}$$

Although the basis need not be orthogonal, it admits a spectral decomposition of the identity $\hat{I} = \sum_{j,k} I_{kj} | \varphi_k \rangle \langle \varphi_j |$; considering $\hat{I}$ to act on the left of the null vector in Eq. (2.2), we easily realize that each matrix element $\langle \varphi_j | \hat{v}_i | \varphi_i \rangle$ must vanish. This fact leads to the evolution law

$$M \dot{A} = \frac{i}{\hbar} L A , \tag{2.3}$$

where A is the coefficient vector, L is the Lagrangian matrix with components

$$L_{ji}(t) = \left\langle \varphi_j(t) \left| i\hbar \frac{\hat{\partial}}{\partial t} - \hat{H} \right| \varphi_i(t) \right\rangle \tag{2.4}$$

and M is the space metric with matrix elements

$$M_{ji}(t) = \langle \varphi_j(t) | \varphi_i(t) \rangle . \tag{2.5}$$

It is clear from (2.4) and (2.5) that the diagonal terms of these matrices, respectively, are the Lagrangians $\mathcal{L}_i(\varphi_i(t), \dot{\varphi}_i(t))$ and the norms of each basis state.

Up to this moment no approximation has been made, so that Eq. (2.3) corresponds to the exact dynamics, its solution depending on the predetermined law of motion of the basis $\{ | \varphi_i(t) \rangle \}$. Moreover, if we know in advance that the exact solution of a given Schrödinger equation belongs to a time-dependent subspace $S(t)$, such solution is the restriction of (2.1) to the above subspace with coefficients that evolve according to (2.3), i.e.,

$$\dot{A}(t) = \frac{i}{\hbar} M^{-1}(t) L(t) A(t) . \tag{2.6}$$

In such a situation, it is no longer necessary to demand the full Hilbert space to be a finite-dimensional one, since it is sufficient that the subspace $S(t)$ satisfies this requirement. This fact then induces an approximate procedure, looking for wave functions of the form (2.1), within a time-dependent set of the Hilbert space, that we believe to contain most components of the true state during a

time interval that meets our observational needs. A numerical illustration of such an approximation will be discussed in Sec. IV.

Let us now examine more closely the characteristics of the dynamical rule (2.3). Since it is derived from the Schrödinger equation, it is clear that both the norm

$$\langle \psi \mid \psi \rangle = A^{\dagger} M A \tag{2.7}$$

and the total energy $\mathcal{H}$

$$\mathcal{H} = \langle \psi \mid \hat{H} \mid \psi \rangle = A^{\dagger} H A \tag{2.8}$$

(where H is the time-dependent matrix with components $H_{ij} = \langle \varphi_i \mid \hat{H} \mid \varphi_j \rangle$) are conserved quantities. On the other hand, the metric matrix M satisfies the following properties, which enable us to easily find its law of motion: (i) Hermiticity, $M = M^{\dagger}$; (ii) positive definiteness, since (2.7) ensures $A^{\dagger} M A \geq 0$ for any A vector; (iii) vanishing determinant if and only if the states $\{ \mid \varphi_i \rangle \}$ are linearly dependent; (iv) M is the identity in the subspace $S(t)$ if and only if the basis is orthonormal.

The evolution law of M can be obtained from the norm-conservation condition $(d/dt)\langle \psi \mid \psi \rangle = 0$ for any state $\mid \psi \rangle$ or vector $A(t)$ and Eqs. (2.6) and (2.7). We easily find

$$\dot{M} = \frac{i}{\hbar}(L^{\dagger} - L) \tag{2.9}$$

which indicates that the metric is invariant if and only if the Lagrangian matrix (2.4) is Hermitian; in such a case, it becomes evident that the matrix T with

$$T_{ji} = \left\langle \varphi_j \left| i\hbar \frac{\hat{\partial}}{\partial t} \right| \varphi_i \right\rangle \tag{2.10}$$

is Hermitian itself.

The Hamiltonian matrix (2.8) is time dependent, in general. Its evolution law can be extracted from the energy conservation condition $(d/dt)\mathcal{H} = 0$ and Eqs. (2.6) and (2.8), giving

$$\dot{H} = \frac{i}{\hbar}(L^{\dagger} M^{-1} H - H M^{-1} L) \ . \tag{2.11}$$

Apparently, the right-hand side of (2.10) should not be expected to vanish unless very special symmetries occur; notice that the operator $G = M^{-1} L$ is the generator of the motion (2.6) and that (2.10) actually is

$$\dot{H} = \frac{i}{\hbar}(G^{\dagger} H - H G) \ . \tag{2.12}$$

Now, if the space metric is invariant, G is Hermitian; consequently, Eq. (2.12) is a Heisenberg-like equation of motion for H with G playing the role of a Hamiltonian. Particular choices of the basis set and selected Hamiltonians $\hat{H}$ may yield commuting H and G matrices, in which case H itself is a dynamical invariant.

III. RELATION TO OTHER DYNAMICAL DESCRIPTIONS

It is interesting to notice that the dynamical law (2.3) can be derived from a variational principle. If we consider the Lagrangian associated to the state $\mid \psi \rangle$ in (2.1),

$$\mathcal{L}(\psi, \dot{\psi}) = \left\langle \psi \left| i\hbar \frac{\hat{\partial}}{\partial t} - \hat{H} \right| \psi \right\rangle = A^{\dagger} L A + i\hbar A^{\dagger} M \dot{A} \ , \tag{3.1}$$

the corresponding Euler-Lagrange equation in the space of variables $(A, \dot{A})$ is exactly (2.3). The solution of the latter may be formally expressed as

$$A(t) = \exp\left[i\hbar \int_0^t dt' M^{-1}(t') L(t') \right] A(0) \ , \tag{3.2}$$

and we may recognize several current dynamical descriptions arising as particular cases of the above solution. Let us consider the following situations.

(i) *Time-independent Hamiltonian $\hat{H}$ with orthonormal eigenvectors* $\mid n \rangle$. In this case the evolution operator in (3.2) is the usual propagator $\exp[-(i/\hbar)\hat{H}t]$ of Schrödinger equations that assigns phases $\exp(-iE_n t/\hbar)$ to each initial amplitude $a_n(0)$.

(ii) *Time-dependent Hamiltonian $\hat{H}(t)$ with orthonormal instantaneous eigenvectors* $\mid n(t) \rangle$. One may observe that the Lagrangian matrix L is Hermitian while the space metric M is the identity, thus the evolution operator in (3.2) is unitary. If we consider that at $t = 0$ the system lies at an eigenstate $\mid n_0(0) \rangle$, the evolution law (3.2) gives the amplitudes $a_n(t)$ as

$$a_n(t) = \left[\exp\left[\frac{i}{\hbar} \int_0^t L(t') dt' \right] \right]_{n, n_0} = \exp\left[\frac{i}{\hbar} \int_0^t [\langle n(t') \mid \dot{n}_0(t') \rangle - \delta_{n n_0} E_{n_0}(t')] dt' \right] \ . \tag{3.3}$$

It is clear that the adiabatic approximation including Berry's phase[5] is obtained from (3.3) as one disregards the nondiagonal overlaps $\langle n \mid \dot{n}_0 \rangle$ with n different from n_0. In fact, in such a case the wave function (2.1) takes the form

$$\mid \psi(t) \rangle = \exp\left[\frac{i}{\hbar} \int_0^t \langle n_0(t') \mid \dot{n}_0(t') \rangle dt' - \frac{i}{\hbar} \int_0^t E_{n_0}(t') dt' \right] \mid n_0(t) \rangle \ , \tag{3.4}$$

where

$$\exp\left[-i/\hbar \int_0^t E_{n_0}(t') dt' \right]$$

is the traditional time-dependent phase of the adiabatic approximation and

$$\exp\left[i/\hbar \int_0^t \langle n_0(t') \mid \dot{n}_0(t') dt' \right]$$

is the geometrical contribution commonly denoted as Berry's phase.[5] In this context, we may observe that Berry's description is equivalent to reducing the Hilbert space to the one-dimensional instantaneous subspace generated by $\mid n_0(t) \rangle$.

(iii) *Nonlinear propagation of a coherent state.* It is well known that when an N-particle system is described by a

coherent state at $t=0$, a good short-time approximation to its exact evolution is prescribed by the time-dependent Hartree-Fock method.[1] The determination of the proper phase of the TDHF wave function is due to Lichtner *et al.*,[3] who showed that such phase should be proportional to the action S related to the moving coherent state $|\mathcal{S}(t)\rangle$,

$$S=\int_0^t dt'\langle \mathcal{S}(t')|\hat{L}|\mathcal{S}(t')\rangle \ . \tag{3.5}$$

Consequently, the TDHF wave function reads

$$\begin{aligned}|\psi_{\rm TDHF}(t)\rangle &= \exp(iS/\hbar)|\mathcal{S}(t)\rangle \\ &= \exp(iS/\hbar)U_{\rm TDHF}(t)|\mathcal{S}(0)\rangle \ ,\end{aligned} \tag{3.6}$$

where $U_{\rm TDHF}(t)$ is the nonlinear generator of the self-consistent motion.[1] We then realize that Eq. (3.6) is the particular realization of (2.1) and (3.2) restricted to the instanteous subspace generated by the coherent state $|\mathcal{S}(t)\rangle$.

(iv) *Superposition of coherent states at $t=0$.* Let us assume that the initial wave function corresponds to a superposition of a finite number of coherent states $|\mathcal{S}_i(0)\rangle$. Suzuki[4] proposed a representation of a semiclassical propagator that assigns the following structure to the time-dependent wave function:

$$|\psi_S(t)\rangle=\sum_j a_j(0)\exp(iS_j/\hbar)|\mathcal{S}_j(0)\rangle \ , \tag{3.7}$$

where S_j is given by (3.5) with the TDHF coherent state $|\mathcal{S}_j(t)\rangle=U_{\rm TDHF}|\mathcal{S}_j(0)\rangle$.

Once again we realize that this dynamical law is a special case of the general one expressed by Eqs. (2.1) and (3.2), that corresponds to the neglect of the nondiagonal elements of the space metric M and the Lagrangian L in the latter. The accuracy of such an approximation cannot be guaranteed in advance in view of the nonorthogonality of the coherent states.[6,7] In particular, the conservation of the norm and the energy should be subjected to a special test for each selection of the initial superposition. This fact can be visualized as follows: The evolution law in (3.7) corresponds to the particular realization of (2.6) that reads

$$\dot{A}(t)=\frac{i}{\hbar}M_d^{-1}(t)L_d(t)A(t) \ , \tag{3.8}$$

where $M_d(t)$ and $L_d(t)$ are the diagonal parts of the matrices M and L; notice that M_d is the identity if the coherent states $|\mathcal{S}_i(0)\rangle$ are normalized. If we evaluate the time derivative of the norm $\langle\psi_S(t)|\psi_S(t)\rangle=A^\dagger MA$ and require it to vanish, employing (3.8) we reach the following condition:

$$A^\dagger(\dot{M}-i[L_d,M])A=0 \ . \tag{3.9}$$

We then recognize that the norm of the wave function is conserved only under very special conditions that involve the selection of the coherent states $|\mathcal{S}_i(0)\rangle$, which determine both the space metric M and the Lagrangian L_d. A similar analysis can be carried upon the energy leading to similar conclusions. By contrast, norm and energy conservation are guaranteed (cf. Sec. II) if the full matrix M and L participate in the dynamics. This fact leads to the approximate dynamics that we illustrate in Sec. IV.

IV. ILLUSTRATIONS

We are particularly interested in the application of our method to a two-level N-fermion system. The most general Hamiltonian that includes two-body interactions can be written in terms of the generators (J_+,J_-,J_z) or (J_x,J_y,J_z) of the SU(2) algebra as[8-10]

$$H=\mathbf{\Omega}\cdot\mathbf{J}+\tfrac{1}{2}\mathbf{J}\alpha\mathbf{J} \tag{4.1}$$

and the moving frame is expanded by a set of coherent states,

$$|\mathcal{S}_i\rangle=\frac{1}{[1+|\mathcal{S}_i|^2]^J}e^{\mathcal{S}_iJ_+}|0\rangle \ . \tag{4.2}$$

In the last expression, $|0\rangle$ is the unperturbed fermionic ground state and the representation label J takes the value $N/2$; the complex variables $\mathcal{S}_i$ are related to the angular coordinates on the Bloch sphere with radius J by

$$\mathcal{S}_i=t_g\left[\frac{\theta_i}{2}\right]e^{-i\varphi_i} \ . \tag{4.3}$$

The predetermined law of motion $|\mathcal{S}_i(t)\rangle$ is given by the TDHF dynamics, whose phase diagrams for quadratic Hamiltonians of the type (4.1) have been widely investigated.[9-11]

We select an initial wave function built as a superposition of n [$n\leq N+1$, $N+1$ being the dimension of the ground-state SU(2) multiplet] coherent states [Eq. (4.2)]. Since different TDHF orbits do not cross, a choice of n linearly independent states $|\mathcal{S}_i(0)\rangle$ guarantees linear independence throughout the time evolution,

$$\sum_{i=1}^n\lambda_i|\mathcal{S}_i(t)\rangle=U^{\rm HF}(t)\sum_{i=1}^n\lambda_i|\mathcal{S}_i(0)\rangle=0 \tag{4.4}$$

if and only if $\lambda_i=0$ for any i. In such a case, one can assert that the metric matrix M is invertible at all times as demanded by the evolution law (3.2). For the sake of a numerical illustration, we adopt the realization of the Hamiltonian (4.1) with $\mathbf{\Omega}=(0,0,\varepsilon)$ and $\alpha_{xz}=\alpha_{zx}=\chi/(N-1)$, where every other coefficient α_{ij} vanishes. In previous works[9,10] we have demonstrated that the TDHF flow is given by the intersection of the Bloch sphere and the quadrics in J space defined by the mean value of expression (4.1) evaluated with respect to the coherent state. In the case under consideration, the quadrics are hyperbolic cylinders;[9,10] the phase flow for $N=6$ can be appreciated in Figs. 3 and 4 of Ref. 9 for a strength $\chi=0.9$ and $\chi=1.5$, respectively.

The essential aspects of the dynamics (3.2) restricted to n coherent states can be appreciated as we consider the overlap $|\langle\psi(t)|\psi_E(t)\rangle|$ between the approximate and the exact wave function for $n=2$. Figures 1–3 display the given overlap as a function of time for the choices of initial conditions drawn at the upper right corner of each plot, together with the overlap between Suzuki's wave function (3.7) and the exact one. The parameters of this calculation are $\chi=1.5$ and $N=6$; it is clear that the linear independence of the evolving coherent states is

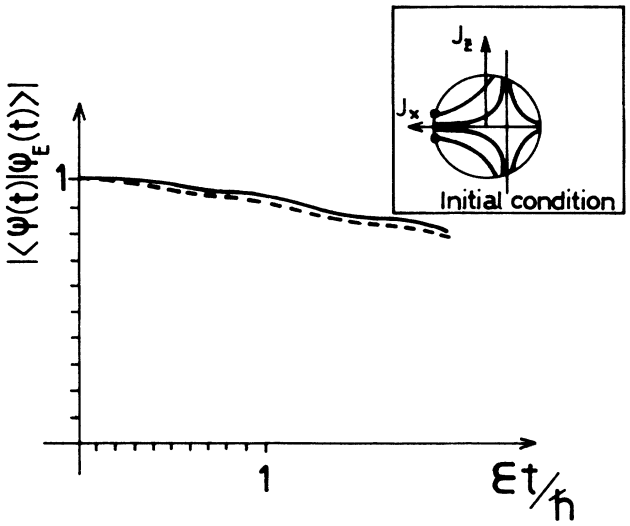

FIG. 1. Overlaps between the exact and the approximate wave functions corresponding to Eq. (3.2) (solid lines) and to Suzuki's approximation (dashed lines), expanded on two ($n=2$) coherent states, as a function of time. The initial conditions are indicated on the upper right corner.

guaranteed since they are different at $t=0$. The major characteristic of this sequence of figures is the progressive departure between the curves as time proceeds; this departure is unobservable in the current scale in Fig. 1 and becomes substantial in Fig. 3. The whole sequence shows that the approximate wave function expanded in the moving basis yields a better approximate to the modulus of the exact one than the wave function that evolves with Suzuki's propagator. This is a general feature of these two alternative descriptions that reproduces itself to different extents over a large sample of initial conditions; it should then call our attention to the inaccuracy of disregarding off-diagonal contributions to dynamical matrices, as discussed at the end of Sec. III.

The above observation can be enforced as we consider the dynamical invariants such as the total energy and the

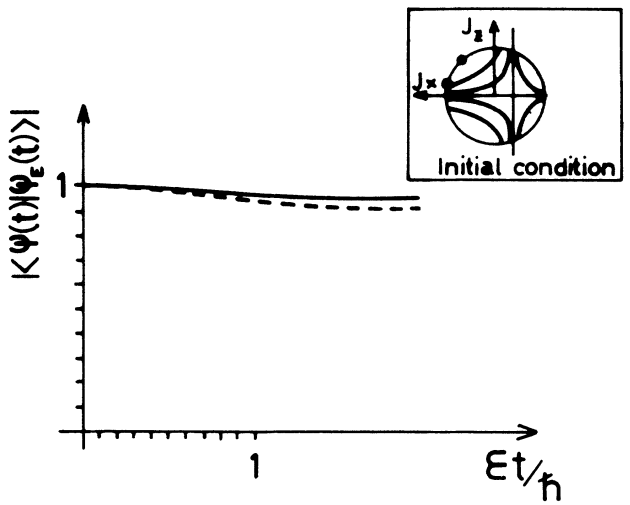

FIG. 2. Same as Fig. 1 for different initial conditions.

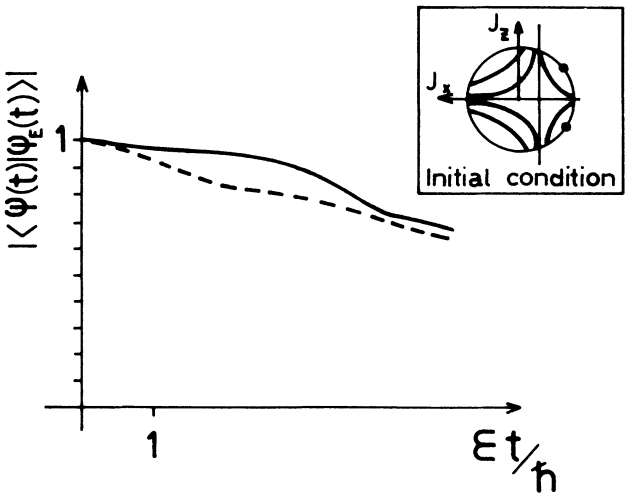

FIG. 3. Same as Fig. 1 for different initial conditions.

norm. Figures 4 and 5 display the energies as functions of time corresponding to Figs. 1 and 2, respectively, and in Fig. 6 we plot the normalization factor $\langle\psi|\psi\rangle$ of the approximate wave functions in Fig. 3. These drawings clearly exhibit the importance of the full Lagrangian and metric matrices as compared to their diagonal restrictions [cf. Eq. (3.8)]; furthermore, the whole set of data here presented strongly recommends the use of the dynamical law (3.2) as an approximation to the exact dynamics.

V. CONCLUSIONS

The numerical analysis of the equation of motion (2.6) [equivalently, (3.2)] for a particular N-particle system under the most simplified choice of an expansion set, namely, two independent coherent states that undergo a TDHF evolution, brings into evidence the benefits that the current method may provide. One realizes that a reasonable approximation to the exact wave function, together with excellent conservation of both the norm and energy, can be achieved during a large time interval as compared to the unperturbed period $\hbar/\epsilon$. By contrast, the goodness of such a description is considerably lowered if one further simplifies the approximate dynamics and disregards the off-diagonal matrix element in the Lagrangian and metric matrices; in particular, the

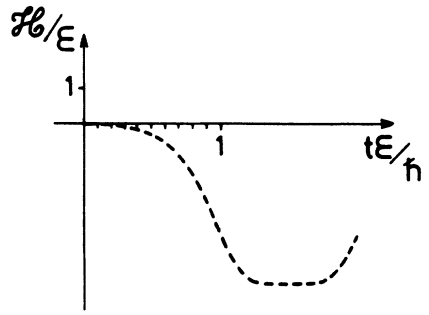

FIG. 4. Approximate energies on the conditions of Fig. 1.

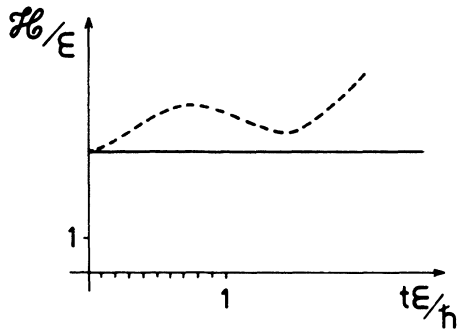

FIG. 5. Approximate energies on the conditions of Fig. 2.

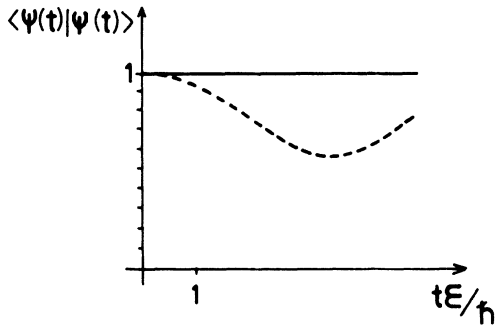

FIG. 6. Normalization of the approximate wave functions in Fig. 3.

dynamical invariants may be destroyed to a large extent.

One might thus wonder whether a full variational description, where one submits both the evolution of the expansion coefficients and the motion of the basis orbitals to the corresponding Euler-Lagrange equations, could improve the description. In other words, one may think of giving up a predetermined law of motion $|\varphi_i(t)\rangle$ and extract a dynamics for the whole collection of variational parameters $\{a_i(t), |\varphi_i(t)\rangle\}$. On the one hand, such a procedure doubles the dimension of the parameter space, which in turn gives rise to a much more complicated problem; on the other hand, one can prove that the matrix in front of the time derivatives [cf. Eq. (2.3)] may become noninversible, a fact that invalidates the treatment. It is then more convenient, for safe applications, to rely on a previously established dynamics for the moving basis.

Along this direction, we can point out the following examples. In the first example, we recall that a numerical TDHF calculation of a collision between two ^{4}He nuclei[12] parametrized by an initial impact parameter develops important variations in the size of the angular momentum dispersion as time elapses. It is then of interest to select an initial condition consisting of a beam of TDHF states, whose dynamics is known from the previous calculations, and investigate to what extent those large fluctuations can be smoothed away. Another example of interest is the case in which the Lagrangian [Eq. (2.4)] in the adiabatic basis is a time-independent matrix; if this happens, the evolution law (2.3) becomes a Schrödinger-like equation with a new Hamiltonian $H=-L$. Diagonalization of this matrix then yields the coefficients of the exact wave-function expansion. This situation takes place, for instance, as one considers a spin-$-\frac{1}{2}$ system in a rotating magnetic field.

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