DISSIPATIVE DYNAMICS OF LARGE AMPLITUDE COLLECTIVE MOTION

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In the paper a theory of dissipative dynamics of nuclear collective motion, based on the projected time dependent Schrödinger equation is formulated. A collective subspace is defined by means of group theoretical methods. Within this subspace an extension of the time dependent Hartree-Fock approach appropriate for dissipative phenomena is proposed.

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The theory of large amplitude nuclear collective motion is not well established yet. The main difficulties are due to the non-unitary and non-linear effects involving many mathematical and conceptional problems which must be solved [4–8]. We propose a theory based on the generalized master equation with an appropriately defined collective subspace by means of group theoretical methods. It is a great advantage of group theory that it allows one to develop a general method for the solution of the equation of motion. The possibility for semiclassical approximations and their generalizations is opened. To achieve this goal, a new variational principle is introduced to find the projected wave function in the semiclassical approximation. The theory is constructed for the many-fermion system, but no special objections exist to use it in the boson case, if the corresponding group defining a collective subspace is compact (an extension to a non-compact case is also possible but requires more advanced methods of the harmonic analysis on groups [9, 10]).

1. The evolution equation of "subdynamics"

Assume a time independent many-body hamiltonian, H, of a closed many-fermion system and two projectors P and Q satisfying the following conditions

$$P+Q=1 \quad \text{and} \quad P\cdot Q=0. \tag{1}$$

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Using the standard projection technique [1–2] and Ref. [4] we obtain the "subdynamics evolution equation" (SEE) for the projected wave function $|\psi_P(t)\rangle \equiv P|\psi(t)\rangle$:

$$i\frac{\partial}{\partial t}|\psi_P(t)\rangle = PHP|\psi_P(t)\rangle + \int_0^t \hat{g}(\tau)\,|\psi_P(t-\tau)\rangle d\tau \tag{2}$$

where

$$\hat{g}(\tau) \equiv -iPHQe^{-iQHQ\tau}QHP \tag{2a}$$

and

$$|\psi_P(0)\rangle = |\psi(0)\rangle \equiv |\mathfrak{C}\rangle. \tag{2b}$$

The initial condition (2b) allows us to neglect in the derivation of SEE the term which describes the influence of initial data on $|\psi_Q(t=0)\rangle \equiv Q|\psi(t=0)\rangle$ on the subsequent time evolution of the system. Equation (2), when applied to the projected density operator ϱ_P instead of the wave function $|\psi_P\rangle$, is sometimes referred to as the pre- or generalized master equation. It has been investigated by Prigogine and his collaborators, see Ref. [3] since the mid-1950's. It was found that Eq. (2) is equivalent to the Schrödinger equation. In addition, it allows us to get an insight into dissipative processes between the P and Q spaces. The time integration in the second term (the "memory" term) of the right hand side of the SEE indicates that the value of $|\psi_P(t)\rangle$ at time t will depend on the past history of the system; the equation is nonlocal in time i.e. nonmarkovian. Moreover, it is obvious that the projected wave function $|\psi_P\rangle$ is not normalized. Its norm is a function of time and describes a contribution of the motion in the P-space to the total evolution of the many-body system i.e. the norm $\|\psi_P(t)\|$ can be understood as a damping function for the P-space motion.

If the P-space is assumed as a collective subspace and the Q-space describes the intrinsic degrees of freedom, we see that SEE is a basic equation for non-adiabatic collective dynamics. Clearly, in the first order of approximation the adiabatic theory can be obtained. This adiabatic approximation is based on the belief that the memory term in SEE can be practically neglected. But in many cases it is not a satisfactory assumption, e.g. for large amplitude nuclear collective motion [4–8].

2. *The definition of the P-space*

To develop a theory of subdynamics based on SEE, the first essential step is the construction of a P-space which, to be useful, should satisfy the following conditions:

- The definition should be general enough to describe a wide class of possible motions.
- The symmetries imposed by the nature of the collective motion should be conserved.
- No redundant variables ought to be introduced such as it is the case e.g. in the generator coordinate method.
- The P-space should be defined in such a way that we can find a method of solving equation (2).

— In addition, for consistency with other approaches, we require to have a possibility to generalize semiclassical approximations in a systematic way, such as e.g. the TDHF theory.

The appropriate definition of the P-space is described in the following: different kinds of collective motion (and in many cases also non-collective ones) can be imagined as "deformations" of the initial configuration, $|\mathfrak{C}\rangle$, of a many-body system. We assume that all the "deformations" form a s-dimensional Lie group G; let us denote by $T(\beta)$, where $\beta \in G$, an unitary representation of the group G in the space of physical states. Any vector, e.g. $|\psi_P(t)\rangle$, belonging to the P-space can now be written as a combination of all possible deformations of the initial state vector $|\mathfrak{C}\rangle$ (if the following integral is well defined [9a, 10])

$$|\psi_P(t)\rangle = \int_G d\beta \phi(\beta, t)^* |\beta\rangle \tag{3}$$

where $\phi(\beta, t)$ is a square-integrable complex function on the group manifold for each moment of time, i.e. $\int_G d\beta |\phi(\beta, t)|^2 < \infty$. $\int_G d\beta$ is an appropriate left-invariant integral defined on the group G, and $|\beta\rangle \equiv T(\beta)|\mathfrak{C}\rangle$. Substitution of the ansatz (3) into SEE gives the equation for the Laplace transform of the function $\phi(\beta, t)$:

$$\int_G d\beta \tilde{\phi}(\beta, z)^* \mathscr{H}(z) |\beta\rangle = i|\mathfrak{C}\rangle \tag{4}$$

with the following "effective hamiltonian"

$$\mathscr{H}(z) \equiv zP - PHP - \tilde{\tilde{g}}(z). \tag{5}$$

The tilde indicates the Laplace transform, e.g.

$$\tilde{\tilde{g}}(z) = \int_0^\infty e^{izt} \hat{g}(t) dt = PHQ \frac{1}{z - QHQ} QHP \tag{6}$$

and the asterisk stands for complex conjugation. For the compact group G (extension to the locally-compact case is also possible) the Peter-Weyl theorem [9b] allows us to transform equation (4) to a system of algebraic linear equations

$$\sum_{\mu pq} f_{pq}^{\mu}(z)^* c_q^{\mu} \frac{\langle e_s^{\nu} | \mathscr{H}(z) | e_p^{\mu} \rangle}{\dim(\mu)} = i \langle e_s^{\nu} | \mathfrak{C} \rangle \tag{7}$$

where

$$f_{pq}^{\mu}(z)^* = \dim(\mu) \int_G d\beta \tilde{\phi}(\beta, z)^* D_{pq}^{(\mu)}(\beta)$$

are the coefficients in the expansion of the function $\tilde{\phi}(\beta, z)^*$ in the series of the matrix elements $D_{pq}^{(\mu)}(\beta)$ of all nonequivalent irreducible representations (μ) of the group G; $\dim(\mu)$ denotes the dimension of the i.r. (μ). The vectors $|e_s^{\mu}\rangle$ $(s = 1, 2, \ldots, \dim(\mu))$ furnish an

appropriate basis for the i.r. (μ) and c_q^μ are the expansion coefficients of the initial state vector $|\mathfrak{C}\rangle$ into this basis. Note, that only residues of the function $f_{pq}^\mu(z)$ must be found to calculate the function $\phi(\beta, t)$, and finally to solve the Eq. (2).

3. *A semiclassical approximation*

The assumption of a sharply peaked function $\phi(\beta', t)$, i.e. semiclassical motion, for each moment of time with the peak at $\beta' = \beta(t)$ ($\beta(0) = e$, where $e \in G$ is the identity element) suggests the following ansatz for the weight function $\phi(\beta', t)$

$$\phi(\beta', t) = W[\beta(t); t]\chi(\beta^{-1}(t)\beta'), \tag{8}$$

where $\chi(\beta'')$ is a peaked function at $\beta'' = e$, and $0 \leqslant W[\,;\,] \leqslant 1$ denotes the norm of the resulting state vector of the "mean motion". The last statement is a consequence of Eq. (2b) which implies that

$$\int_G d\beta' \chi(\beta')\,|\beta'\rangle = |\mathfrak{C}\rangle. \tag{9}$$

From Eqs. (8) and (3) we obtain a semiclassical approximation of the projected wave function

$$|\psi_P(\beta(t), t)\rangle = W[\beta(t); t]\,|\beta(t)\rangle, \tag{10}$$

where

$$|\beta(t)\rangle = T(\beta(t))\,|\mathfrak{C}\rangle.$$

With equation (10) we restrict ourselves to an orbit (in the group theoretical sense) of the initial state vector like in the HF or TDHF calculations where only the orbit of the Slater determinants (with respect to a unitary group [11]) are taken into account. However, it must be emphasized that the ansatz (10) is much less restrictive than the TDHF approach. Moreover, for an appropriate choice of the group G it should give an exact form of the "mean motion" of the many-body system. Obviously, it makes sense only if $\phi(\beta, t)$ is a sharply peaked function. From SEE and Eq. (10), a little algebra and integration from $t = 0$ to an arbitrary t_0 yield an expression which allows us to postulate a variational principle for the calculation of $W[\beta(t); t]$ and $|\beta(t)\rangle$ separately:

$$i \ln W[\beta(t_0); t_0] = \int_0^{t_0} dt' \left\{ \langle\beta(t')|\, PHP - i\frac{d}{dt'}\,|\beta(t')\rangle \right.$$

$$\left. + \int_0^{t'} d\tau \frac{W[\beta(t'-\tau), t'-\tau]}{W[\beta(t'), t']} \langle\beta(t')|\hat{g}(\tau)\,|\beta(t'-\tau)\rangle \right\}. \tag{11}$$

We assume that the collective path is defined by a critical (stationary) damping function $W[\beta; t]$ (i.e. one which is stationary with respect to small variations of $|\beta\rangle$ at each time). Clearly, the physical nature of this postulate must be carefully discussed in the future.

At this moment we note only that it is fulfilled for the adiabatic case, $W = \text{const.}$, and is expected to be true for small deviations from adiabaticity. The critical point technique is more suitable for the group transformations than the standard variational calculus [11]. To apply this method we deform the vector $|\beta(t)\rangle$ by the set of all possible one-parameter subgroups of G. Because we need these subgroups only in a small neighbourhood around the identity $e \in G$, we can write

$$G_Y(t) \equiv e^{\alpha Y(t)}, \tag{12}$$

where α is a small real parameter and $Y(t)$ is an arbitrary skew-symmetric operator belonging to the Lie algebra of G. Transforming with the operator of Eq. (12) one obtains from Eq. (11)

$$i \ln W[e^{\alpha Y(t)}\beta; t] = \int_0^{t_0} dt' \left\{ \langle \beta(t') | e^{\alpha Y(t')^+} \left(PHP - i \frac{d}{dt'} \right) e^{\alpha Y(t')} | \beta(t') \rangle \right.$$

$$\left. + \int_0^{t'} d\tau \frac{W[e^{\alpha Y(t')}\beta; t'-\tau]}{W[e^{\alpha Y(t')}\beta; t']} \langle \beta(t') | e^{\alpha Y(t')^+} \hat{g}(\tau) e^{\alpha Y(t')} | \beta(t'-\tau) \rangle \right\}. \tag{13}$$

We now differentiate Eq. (13) with respect to α and use the fact that $Y(t') = \sum_{k=1}^{s} A_k(t') Y_k$, where Y_k is a skew-symmetric basis (independent of time) of the Lie algebra of G and $A_k(t')$ are arbitrary functions of time satisfying the following condition

$$A_k(0) = A_k(t_0) = 0, \quad k = 1, 2, \ldots, s. \tag{14}$$

(Relation (14) is chosen in analogy to the standard conditions for variations in the case of fixed initial and final points.) Because the resulting equation must be fulfilled for all functions $A_k(t')$ consistent with Eq. (14), we obtain a set of s equations

$$i \frac{d}{dt} \langle \beta(t) | Y_k | \beta(t) \rangle = \langle \beta(t) | [Y_k, PHP] | \beta(t) \rangle$$

$$+ (-1) \int_0^t d\tau \frac{W[\beta, t-\tau]}{W[\beta, t]} \langle \beta(t) | [\hat{g}(\tau), Y_k] | \beta(t-\tau) \rangle. \tag{15}$$

Eqs. (11) and (15) provide a system of $s+1$ coupled equations for $|\beta(t)\rangle$ and $W[\beta(t); t]$. In the limit of weak coupling between P- and Q-spaces it is expected that the ratio $W[\beta; t-\tau]/W[\beta; t] \approx 1$ for $0 \leqslant \tau \leqslant t$. Equations (15) become then decoupled from Eq. (11). Neglecting the memory kernel in Eq. (15) and assuming that G is an unitary group of dimension s with the generators

$$Y_k = \begin{cases} a_\mu^+ a_\nu - a_\nu^+ a_\mu \\ i(a_\mu^+ a_\nu + a_\nu^+ a_\mu) \end{cases} \qquad \nu, \mu = 1, 2, \ldots, n$$

we obtain after a few simple transformations an equation of motion for the one-body density in P-space

$$i\frac{d}{dt}\langle\beta(t)|a_\mu^+ a_\nu|\beta(t)\rangle = \langle\beta(t)|\,[a_\mu^+ a_\nu, PHP]\,|\beta(t)\rangle.$$

Choosing the initial state $|\mathfrak{C}\rangle$ as a Slater determinant and factorizing the two-body density into an appropriate product of one-body densities [12] end up with the TDHF equations (assuming that PHP is a sum of one- and two-body operators). Other choices like e.g. linear combinations of Slater determinants lead to an extension of TDHF. Corrections due to a coupling between P- and Q-space are described by the memory kernel in Eq. (15) and have to be included in any microscopic theory of non-adiabatic phenomena. Much present and future activities are devoted to studies of various approximations for the memory kernel.

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