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Adiabatic Time Dependent Hartree-Fock Theory

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1. Introduction

Many sorts of large amplitude collective phenomena have the very characteristics, that there are certain classical parameters $q_i(t)$, whose evolution in time is intimately connected with the time evolution of the total A-body system during the collective process. Typical parameters of this sort are e.g. necking and elongation in case of fission, the distance of the ions in a heavy ion reaction, the multipole moment in a multipole vibration. Already in the early days of nuclear physics this feature gave rise to theories which tried to describe those processes by means of a collective Schrödinger equation. This concept is obviously based on the assumption that the collective degrees of freedom are in some way describable by the parameters q_i and that they are to some extent decoupled from the other, i.e. intrinsic degrees of freedom.

In an actual microscopic calculation one usually proceeds in four steps: (For simplicity we will assume only one q(t))

1) One guesses a collective path. This is understood to be a set of time independent A-body wave functions $|q\rangle$ characterized by q as parameter. Typical choices are Slater determinants composed out of single particle functions of a parametrized Saxon-Woods potential. Another possibility con-

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sists in the use of CHF techniques. For small colliding systems often displaced Gaussians or harmonic oscillator functions are used.

2) Using $|q\rangle$ one calculates a potential energy surface as expectation value of the total Hamiltonian, assuming an appropriate two body interaction:

$$V(q) = \langle q|\hat{H}|q\rangle \tag{1}$$

3) Along the collective path $|q\rangle$ one calculates the collective mass M(q). There are various microscopic descriptions in the literature, e.g. the cranking model, the approach of Thouless and Valatin, the generator coordinate method, or the adiabatic time dependent Hartree-Fock approach in the way formulated by Brink, Giannoni and Veneroni. With the mass $\mathcal{M}$ and the collective potential $\mathcal{V}$ one writes then down a classical collective Hamiltonian for the considered motion

$$H_c(q,p) = \frac{p^2}{2\mathcal{M}(q)} + \mathcal{V}(q) \tag{2}$$

where $p = \mathcal{M}(q)\,\dot{q}$.

4) The last step consists in quantizing eq. (2), often just by replacing $p \to -id/dq$, which gives then a collective Schrödinger equation.

Such a procedure contains several inconsistencies: a) There is a great deal of arbitrariness in guessing the collective path. The choices suggested by no means guarantee that along the path the collective and intrinsic degrees of freedom are decoupled such that they allow a separate treatment of the collective channel. Hence it is desirable to have a theory which determines the collective path by making explicitly use of such a decoupling condition, rather than guessing the path. b) Collective mass and collective path should not be determined by different models since they are closely

related to each other. The dynamics of the moving system determines both quantities simultaneously and the collective path is certainly influenced by the variation of the mass along the path and also of the collective potential along the path. Hence one should have a system of coupled equations which determine simultaneously the path and the mass. c) The third inconsistency is related to the quantization procedure. Certainly $p \to -id/dq$ is too naive since one knows that it is wrong. Hence one would like to have a clear prescription how to quantize H_c without ambiguities. The GCM and RGM, of course, have no problems in deriving the Schrödinger equation, since they are quantized theories from the beginning. So one could use the collective path directly in GCM and RGM without calculating explicitly a collective mass and without bothering about a quantization. However we do not know if such a procedure is correct since the example of uniform translation tells us that the mass of GCM might not be always correct. We remember that such considerations led to the introduction of the double projection method. Hence it is desirable to have a theory, which

1) selects by itself the relevant collective degrees of freedom, i.e. determines the collective path rather than guessing it
2) calculates consistently with the path a collective mass $\mathcal{M}(q)$ and a collective potential $\mathcal{V}(q)$ leading to a classical Hamiltonian (adiabatic)

$$H_c = \frac{p^2}{2\mathcal{M}(q)} + \mathcal{V}(q)$$

3) quantizes unambiguously the classical H_c in order to obtain a quantum-mechanical H_c with

$$H_c = -\frac{d}{dq}\frac{1}{2M(q)}\frac{d}{dq} + V(q)$$

4) provides a clear interpretation of the collective wave function by calculating matrix elements of obserables.

We will see that one can formulate such a theory[1] if one restricts oneself to collective paths consisting out of Slater-determinants. The corrsponding equations of motion are the TDHF equations which will be used in their adiabatic limit. Further details of the model will be found in ref. 1).

2. The ATDHF-theory

The TDHF approach is essentially characterized by the equation, all involving the single particle density matrix ρ:

$$i\dot{\rho} = [W,\rho] \qquad W = T + \mathrm{Tr}\, v\, \rho \tag{1,2}$$

$$\rho^2 = \rho = \rho^+ \quad \mathrm{Tr}\, \rho = A \qquad \dot{A} = 0 \tag{3}$$

$$E = \mathrm{Tr}\, T\rho + \frac{1}{2}\, \mathrm{Tr}\, \mathrm{Tr}\, \rho\, v\, \rho \qquad \dot{E} = 0 \tag{4}$$

For an adiabatic formulation of TDHF we perform an expansion

$$\rho(t) = \rho_0(t) + \rho_1(t) + \rho_2(t) \ldots \tag{5}$$

about the (yet unknown) collective path:

$$\rho_0(t) = \rho_0(q) \quad \text{with} \quad q = q(t) \tag{6}$$

The first order correction should come from the velocity and is assumed to have the structure

$$\rho_1(t) = \dot{q}\, \bar{\rho}_1(q) \tag{7}$$

If one iserts expansion (5) into E of eq. (4) one obtains eventually a kinetic energy

$$K = \frac{1}{2}\mathcal{M}(q)\, \dot{q}^2 \tag{8}$$

and a potential energy

$$\mathcal{V}(q) = \mathrm{Tr}\, T\rho_0 + \frac{1}{2}\, \mathrm{Tr}\, \mathrm{Tr}\, \rho_0\, v\, \rho_0 \tag{9}$$

whose sum is a classical Hamiltonian with $p = \mathcal{M}(q)\,\dot{q}$,

$$E = \mathcal{H}_c(q,p) = \frac{p^2}{2\mathcal{M}(q)} + V(q) \tag{10}$$

By means of the equations of motion to be derived, one can write

$$\mathcal{M}(q) = i\,\mathrm{Tr}\,\{[\rho_0,\bar{\rho}_1]\;\partial_q\,\rho_0\} \tag{11}$$

The essential question is now, how one can obtain $\rho_0(q)$ and $\bar{\rho}_1(q)$, both quantities being essential for the dynamics. In order to perform a perturbation expansion of the TDHF equations we write

$$W = H_0 + W_1 + W_2 + F + \ldots \tag{12}$$

where the F is introduced solely on the ground for convenience, namely to have the derived ρ_0 as eigenvolution of H_0. F is unknown and has to be determined. One obtains now a hierarchy of equations:

$$[H_0,\rho_0] = 0 \qquad \propto \dot{q}^0 \tag{13a}$$

$$[H_0,\rho_1] + [W_1,\rho_0] = i\dot{\rho}_0 \qquad \propto \dot{q}^1 \tag{13b}$$

$$[H_0,\rho_2] + [W_2,\rho_0] + [W_1,\rho_1] + [F,\rho_0] = i\dot{\rho}_1 \tag{13c}$$

Eq. (13) are yet only a rewriting of TDHF, not yet equations to derive a path. For the following one has to clear an essential conceptional point: We are interested in ATDHF as a tool to derive a collective Hamiltonian H_c from it. This one, of course, should be the same for a range of energies of the collective states. This means the H_c describing e.g. a zero phonon state and the H_c describing the two phonon state should be identical, otherwise there would be a strong coupling between intrinsic and collective motion and the concept of a collective Hamiltonian would break down. This has as consequence, that only those TDHF trajectories $\rho(t)$ can be used to extract the

collective path ρ_0, which are stable against a variation of the initial energy, or equivalently in the collective channel, a variation of $\dot{q}$. Hence, we must treat $\dot{q}$ as a free parameter, and then our equations are bound to calculate us the collective path.

With $\dot{q}$ as free parameter eq. (13c) splits into two equations which have to be fulfilled independently, viz. a contribution from $\dot{q}^0$ terms, which determines together with eqs. (13a, 13b) the ρ_0 and $\bar{\rho}_1$

$$[F,\rho_0] = -i \frac{\partial \mathcal{V}}{\partial q} \bar{\rho}_1 \tag{14}$$

and a second order equation, which determines the p-h elements of ρ_2. These elements should be small, if the approach is valid, and hence the following eq. (15) can be used as criterion for the validity[2] of ATDHF

$$[H_0,\bar{\rho}_2] + [\bar{W}_2,\rho_0] + [\bar{W}_1,\bar{\rho}_1] = i \sqrt{\mathcal{M}}\, \partial/\partial q \, (\bar{\rho}_1/\sqrt{\mathcal{M}}) \tag{15}$$

After introducing the operator $\hat{Q}$ by $F = \lambda\hat{Q}$ and $\lambda = \partial\hat{Q}/\partial q$ one obtains after some formal operations the final set of equations, which determines simultaneously $\rho_0(q)$, $\bar{\rho}_1(q)$, $\mathcal{M}(q)$ and together with eq. (9) also $\mathcal{V}(q)$:

$$[W_0 - \lambda\hat{Q},\rho_0] = 0 \tag{16a}$$

$$[W_0,\bar{\rho}_1] + [\bar{W}_1,\rho_0] = i\, \partial\, \rho_0/\partial_q \tag{16b}$$

$$\mathcal{M}(q) = i\, \mathrm{Tr}\, \{[\rho_0,\bar{\rho}_1]\, \partial\, \rho_0/\partial_q\} \tag{16c}$$

$$\hat{Q} = \frac{i}{\mathcal{M}} [\rho_0,\bar{\rho}_1] \tag{16d}$$

The Q has the remarkable property

$$\rho(qp) = \rho_0(q) + ip\, [\hat{Q},\rho_0] \tag{17}$$

One also can introduce an operator $\hat{P}$ by

$$[\hat{P},\rho_o] = i\frac{\partial\rho_o}{\partial q} \tag{18}$$

which is weakly conjugate to $\hat{Q}$:

$$\mathrm{Tr}\,\{[\hat{Q},\hat{P}]\rho_o\} = i \tag{19}$$

The equations (16) can be solved in different ways[1], the easiest of them will be described here: Suppose one starts with an initial guess for the CHF-operator $\hat{Q}$. Then one can determine ρ_o by solving eq. (16a) and $\bar{\rho}_1$ by solving eq. (16b). The mass can be evaluated readily, eq. (16c), and also a new $\hat{Q}$, eq. (16d). This new $\hat{Q}$ may be inserted into eq. (16a) in order to obtain a new $\rho_o(q)$, etc. until convergence.

3. The quantization

For the quantization we can exploid the fact, that by assumption there exists a canonical transformation from the 3A particle coordinates to intrinsic ones, ξ_i, and a collective one, Q. Hence the total energy, being identical with the classical Hamiltonian

$$\mathcal{H}_c(p,q) = \frac{p^2}{2\mu(q)} + \mathcal{V}(q) = E \tag{20}$$

can be written as

$$\mathcal{H}_c(p,q) = \int d\xi_i\, dQ\, \langle pq|\xi_i Q\rangle\, H(\xi_i,Q)\, \langle\xi_i Q|pq\rangle \tag{21}$$

The collective Hamiltonian H_c is now defined as that quantity, which remains in eq. (21) after averaging over all ξ_i

$$\mathcal{H}_c(q,p) = \int dQ\, \langle pq|Q\rangle\, H_c(Q,P)\, \langle Q|pq\rangle \tag{22}$$

with $P = -i\, d/dQ$. The wave packets $\langle Q|pq\rangle$ and the H_c is still to be determined. We assume H_c to be a local differential operator of 2nd order, then,

since (22) must be valid for any value of q and p

$$\langle Q|pq\rangle = \exp(ipQ)\ \langle Q|q\rangle \tag{23}$$

The $\langle Q|q\rangle$ can be determined now in the following way: The role of Q in the one dimensional Q-space, i.e.

$$\langle Q|pq\rangle_Q \overset{\sim}{=} (1 + ipQ)\ \langle Q|q\rangle \tag{24}$$

and that of $\hat{Q}$ in the 3A-dimensional space

$$\langle x_i|pq\rangle_A = (1 + ip\hat{Q})\ \langle x_i|q\rangle \tag{25}$$

is obviously identical. Hence we are going to identify the moments

$$\langle q|\hat{Q}^n|q\rangle_A = \langle q|Q^n|q\rangle_Q \tag{26}$$

which provides some information about $\langle Q|q\rangle$. This, however, is sufficient to defold the classical $\mathcal{H}_c$, if we assume Gaussian like wave packet

$$\langle Q|q\rangle \propto \exp\left[-\frac{1}{4\Delta Q^2}(Q-q)^2\right] \tag{27}$$

with

$$\Delta Q^2 = \langle q|(Q-q)^2|q\rangle \tag{28}$$

For sufficiently small ΔQ^2 one obtains for a H_c of the form

$$H_c = -\frac{d}{dq}\frac{1}{2M(q)}\frac{d}{dq} + V(q) \tag{29}$$

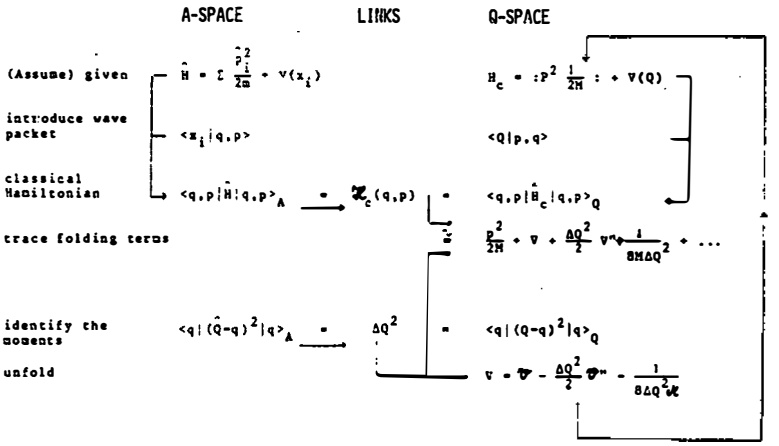
the relations

$$M(q) \simeq \mathcal{M}(q) \tag{30}$$

$$V(q) \simeq \mathcal{V}(q) - \frac{\Delta Q^2}{2}\mathcal{V}''(q) - \frac{1}{8\mathcal{M}\Delta Q^2} - \frac{1}{8}(1/\mathcal{M})'' \tag{31}$$

The assumed structure of the kinetic operator in eq. (29) is by no means

necessary, one can assume any other structure. The resulting collective Hamiltonian, however, after the defolding procedure is identical to eqs. (29,31). This means, neither the kinetic operator nor the collective potential are uniquely determined, but only the sum, i.e. the total collective Hamiltonian. The result is identical to the one obtained by the GCM with GOA, although the masses M are different. This difference will be the subject of a different talk[3]. The logical scheme of the present quantization[1] can be exposed in the following way:



This scheme can obviously be applied to any other operator in A-space: Suppose we are interested in the matrix elements of an operator $D(x_1 \ldots x_\alpha)$ between collective wave functions, i.e. the eigenfunctions of H_c. Then we calculate $\mathcal{D}(q) = \langle q|D|q\rangle_A$ and construct from it the collective operator $D_c(q) = \mathcal{D}(q) - \frac{\Delta Q^2}{2}\mathcal{D}''(q)$. The matrix elements of D are now

$$D_{if} = \int \Psi_c^{(f)*}(q)\, D_c(q)\, \Psi_c^{(i)}(q)\, dq \qquad (32)$$

Hence altogether we have a complete mapping of the A-space into the one-dimensional collective Q-space.

It should be pointed out, that the prescribed quantization procedure is by no means restricted to Slater-determinants. Any theory, which is able to provide $\mathcal{M}(q)$, $\mathcal{V}(q)$ and ΔQ^2 can be quantized in this way. The effect of the terms $\mathcal{E}(q) = V(q) - \mathcal{V}(q)$ in the collective potential is by no means negligible. These zero point corrections lower the collective potential such that the lowest eigensolution of H_c lies below the ground state HF energy. The $\mathcal{E}(q)$ also change the shape of the potential, which in case of fissioning nuclei, lowers sometimes the second barrier by more than 2 MeV which reduces the lifetimes by a factor 10^{-6}.

References

1) K. Goeke and P.-G. Reinhard, Ann. Phys. in press

2) P.-G. Reinhard and K. Goeke, Phys. Lett. 69B (1977) 17

3) P.-G. Reinhard and K. Goeke, preprint 1977

DISCUSSION

H. Hofmann: To my feeling the quantization procedure you described is unique at most up to additive functions of Q whose average over Q vanish.

K. Goeke: You are right!