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The validity of the adiabatic time dependent Hartree Fock theory

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1/. Introduction

The objective of this paper is to examine the validity of the ATDHF theory for the case of fission. The application of the adiabatic theory for fission has a long history [1], the justification of it is that fission motion is characterized by the motion of a few slowly changing parameters. However, the adiabatic treatment does not allow the dissipation of the energy from the fission degrees of freedom, which indicates that it cannot be applied for the whole fission process, the best we can expect that parts of it can be well described by the adiabatic theory.

In the following we deduce the ATDHF equations by re-writing the equations of Villars [2] in coordinate space. The equations we got this way are basically the same as that of Baranger and Veneroni [3] and Brink at al [4], but is more suitable for our purposes. The results of the ATDHF equations will compared with that of the TDHF equations and their applicability for fission will be examined.

2/. Deduction of the ATDHF equations in coordinate space

In the last years successfull attempts were made to solve the TDHF equations in coordinate space [5,6]. The single particle TDHF equations can be written as [5,7]

$$h\,\psi_i(x,t) = i\,\frac{\partial \psi_i(x,t)}{\partial t}\,, \qquad /1/$$

where h is the single particle Hamiltonian and the ψ_i -s are the single particle wavefunctions. In the following we shall consider h which is assumed to be a function of the density only

$$h = t_{kin} + W(\varrho)\,. \qquad /2/$$

Let us assume, that there is a time dependent parameter $q(t)$ which together with its canonical coniugate $p(t)$ uniquely characterizes the time dependence of the system's motion. This is a basic condition for the applicability of the ATDHF approximation, and in reality it is very rarely satisfied. It means that at each time value t_i, when $q(t_i)$ and $p(t_i)$ have the same q_0, p_0 values, the whole system has to be exactly in the same state, so there cannot be energy transition between the different degrees of freedom, for example. If this basic condition in satisfied, the wave function can be written as follows

$$\Psi_i(x,t) = e^{ip(t)\hat{Q}}\,\varphi_i(x,q(t)), \qquad /3/$$

where $\hat{Q}$ is an undefined operator to be determined by the TDHF equations. If $q(t)$ changes slowly in time, we can expand the /3/ wavefunctions up to second order in p

$$\Psi_i(x,t) = \left(1 + ip\hat{Q} - \frac{p^2}{2}\hat{Q}^2\right)\varphi_i(x,q), \qquad /4/$$

The time derivative of $p(t)$ and $q(t)$ can be determined from the cannonical equations [see. Ref.2]:

$$\left.\begin{aligned} \dot{q} &= \frac{\partial \mathcal{H}(p,q)}{\partial p} = \frac{p}{M(q)}, \\ \dot{p} &= -\frac{\partial \mathcal{H}(p,q)}{\partial q} = -\frac{\partial V(q)}{\partial q} + O(p^2), \end{aligned}\right\} \qquad /5/$$

where

$$V(q) = \langle a\Pi_i \varphi_i | H | a\Pi \varphi_i \rangle, \qquad /6/$$

and

$$\mathcal{H}(p,q) = \langle \Phi | H | \Phi \rangle = V(q) + \frac{p^2}{2M(q)}, \qquad /7/$$

is the expectation value of the Hamiltonian between the Slater determinant of the /3/ single particle wavefunctions. To ensure that p is the canonically conjugate variable to q the wavefunctions have to satisfy the condition

$$2\sum_i \left(\hat{Q}\varphi_i, \frac{\partial \varphi_i}{\partial q_\nu}\right) = 1. \qquad /8/$$

Substituting /4/ into /1/, taking into account the /5/ canonical equations, the coefficients of the different p exponents have to be equal to zero. The zeroth and first order coefficients supply the equations

$$h\varphi_i = \lambda(q_\nu)\hat{Q}\varphi_i , \qquad /9/$$

$$h(\hat{Q}\varphi_i) = \frac{1}{M}\frac{\partial \varphi_i}{\partial q_\nu} + \lambda \hat{Q}^2 \varphi_i , \qquad /10/$$

where $\lambda(q_\nu) = \partial V/\partial q_\nu$. /9/-/10/ do not determine uniquely the $\hat{Q}$ operator, because we neglected the higher order terms in p /the higher order coefficients would have given equations for $\hat{Q}^2\varphi$, $\hat{Q}^3\varphi$ etc./ In the adiabatic approximation there is an ambiguity in $\hat{Q}$, which we remove by choosing its matrix elements among the particle states to be equal to zero. With this assumption, using the notation

$$\hat{Q}\varphi_i(x, q_\nu) = A_i(x, q_\nu) + \frac{e_i(q_\nu)}{\lambda(q_\nu)}\varphi_i(x, q_\nu) , \qquad /11/$$

$$S_{ij} = \langle \varphi_j \mid \hat{Q} \mid \varphi_i \rangle$$

/9/-/10/ can be written:

$$h\varphi_i = \lambda A_i + e_i \varphi_i \quad , \qquad /12/$$

$$hA_i = \frac{\lambda}{M}\frac{\partial \varphi_i}{\partial q_\nu} + \lambda \sum_j A_j S_{ij} +$$

$$+ \sum_j \varphi_j \left[e_j S_{ij} + \lambda \langle A_j, A_i \rangle - \lambda \sum_k S_{jk} S_{ki} \right] . \qquad /13/$$

Equations /12/-/13/, together with /6/ and /8/ have to be solved by interation. As a first step we assume for A_i a form $A_i(x, q_\nu) = f(x)\varphi_i(x, q_\nu)$, with this choice the /12/ equations are just the constrained HF equations. However, the constrain operator has to be determined self-consistently by the equations /13/, together with $M(q)$ and $V(q)$ /eqs. /6/ and /8/ /. That is the big advantage of the ATDHF methods of Villars [2]. In our calculation the self consistent procedure converges quite well; from the first to the second step of the interation the value of $V(q)$ does not change too much, only between 10-15 %. However the value of $M(q)$ changed quite significatly, 35-40 %, which shows that the self-consitency must be enforced.

3/. Deduction of the adiabatic parameters from the TDHF equations

Since the ATDHF equations are only approximations of the TDHF equations, one can estimate the validity of the ATDHF equations solving the same problem with both method. For this

reason we examined the fissioning os slabs with both method. The slab geometry and the solution of the TDHF equations for slabs are described in details in Ref. [5], and the fissioning of slabs is described in Ref. [8]. The wavefunctions in the time t=0 can be written as

$$\Phi_n(z, t=0) = \phi_n^{HF}(z)\, e^{iS(z)} \qquad /14/$$

where the ϕ_n^{HF} -s are the static HF wavefunctions and $e^{iS(z)}$ imposes an initial coherent velocity field, $v(z) = \frac{\hbar}{m}\frac{\partial S}{\partial z}$. We considered slab-fission for different initial conditions, oscillations, when $S(z) = \pm \alpha (z - z_0)^2$, Coulomb type of excitations, when $S(z) = \beta^{n,p} |z - z_c|$, and $\beta^{n,p}$ has different sign for neutrons and protons, and collisions of big slabs with small o [illegible], which corresponds to the neutron induced fission. In the last case we did not get fission at all, even for large excitation energies /2 MeV/particle/, in the first two cases above $E^*/A \sim 0.2$ MeV exciation energy however fission occured.

The ATDH approximation is applicable only if we find a q parameter, which together with p describes well enough the time dependence of the system's motions. At the beginning of the fission process in each case the excitation energy strongly dissipates and it is redistributed among the different degrees of freedom. Therefore in this period there is no q parameter which gives a satisfactory description of the motion. However, if fission occurs al all, the last part of the process can be

described almost independently from the inital conditions. Once the slabs start to oscillate, there is not much energy transfer among the different degrees of freedom. The motion can be described then by a q parameter. For slabs, the best choice for q turns out to be

$$\delta = \sqrt{\langle z^2 \rangle} - \sqrt{\langle z^2 \rangle - \langle z \rangle^2}\ , \qquad /15/$$

which gives roughly the average distance of the maximum density places of the fragmenting slabs.

After the choice of q, M(q) and V(q) can be determined from the TDHF equation. Since the ATDHF method determines an M and V for p=0, that is to say in the small excitation energy limit, we have to calculate them for small excitations. The comparison of their values in the two approximations is under investigation.

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References

1./ J.R.Nix, Ann. Rev. Nucl. Sci. 22 /1972/ 65 and see References there;

2./ F.Villars, Nucl.Phys. A285 /1977/ 269;

3./ M.Baranger and M.Véneroni, to be published;

4./ D.M.Brink, M.J.Giannoni and M.Véneroni, Nucl. Phys. A258, /1976/ 237;
Y.M.Engel, D.M.Brink, G.Goeke and S.J. Krieger, Nucl. Phys. A249 /1975/ 215;

5./ P.Bonche, S.Koonin and J.W.Negele, Phys. Rev. C13 /1976/ 1226;

6./ S.E. Koonin, Phys. Lett. 61B /1976/ 227;
S.E.Koonin, K.T.R.Davies, V.Maruhn-Rezwani, H.Feldmeier, S.I.Krieger and J.W.Negele, Phys. Rev. C15 /1977/ 1359;
R.Y.Cusson and J.Maruhn, Phys. Lett. 62B /1976/ 134;

7./ A.Kerman and S.E.Koonin, to be published in Adv. of Physics;

8./ J. Németh, to be published in the Proceedings of Reaction Models'77, Balatonfüred.

DISCUSSION

K. Goeke: Could it be that the failure of the adiabatic approximation in the beginning of your one-dimensional fission process is caused by the fact that you want to use a one-dimensional collective path rather than a two- or three-dimensional?

J. Németh: I do not think so, it is rather due to the fact that with adiabatic approximation one cannot describe the transition of the energy between single-particle and collective degrees of freedom.