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RELATION BETWEEN VARIOUS MICROSCOPIC THEORIES OF COLLISIONS AND NUCLEAR MOTIONS

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INTRODUCTION

The subject covered in this talk is fairly miscellaneous, for it is an attempt to relate several theories, approximations and representations which are currently in use in nuclear physics for a microscopic description of nuclear motion. As will be seen most of the considerations which follow are not restricted to the study of heavy ion collisions. They can be adapted in general to the study of collective motion by transitions between bound states.

In a first section, it will be shown that time can be used as a generator coordinate in order to cure the time-dependent Hartree-Fock (T.D.H.F.) description of nuclear collisions from incorrect boundary conditions. The role of fluctuations in asymptotic regions will be investigated in more detail in a second section, where it will be shown that, just to give an example, the calculation of a fission barrier by means of a constrained Hartree-Fock (C.H.F.) calculation demands some precaution. In a third section, it will be shown how the generator coordinate formalism generates a rigorous definition of effective masses and potentials when an adiabatic limit (A.L.) can be taken. In that limit, it will turn out that there is a significant amount of formal (and not only physical) identity between the Born - Oppenheimer approximation (B.O.A.) and that definition of collective parameters. Finally, section 4 contains a brief remark on the continuity between the channel region and the interaction region, and thus between asymptotic masses and potentials and collective parameters. It also contains, as a conclusion, the proposal that such a continuity might be a guide for a more general, statistical generalization of the low energy theory.

1. TIME AS A GENERATOR COORDINATE

Let $\mathcal{H}$ be the usual nuclear Hamiltonian, sum of the kinetic energy $\mathcal{E}$ and two-body interaction $\mathcal{V}$. At time $t = 0$ we consider a Slater determinant Φ_o, which is arbitrary (it will be made less arbitrary below). For any Slater determinant Φ, it is possible to fold the density of the matter described by Φ with the potential $\mathcal{V}$, take into account exchange terms, and generate the *one-body* Hartree-Fock average field $\mathcal{U}(\Phi)$, thus the Hartree-Fock Hamiltonian $h(\Phi) = \mathcal{E} + \mathcal{U}(\Phi)$.

The time-dependent Schrödinger equation (T.D.S.E.)

$$i\hbar\,\dot{\Psi} = \mathcal{H}\,\Psi \quad , \tag{1}$$

and the T.D.H.F. equation

$$i\hbar\,\dot{\Phi} = h(\Phi)\,\Phi \quad , \tag{2}$$

are both first-order differential equations with respect to time.

Their solutions, respectively $\Psi(t)$ and $\Phi(t)$ are thus completely defined by the initial condition $\Psi(t=0) = \Phi(t=0) = \Phi_o$. Obviously, as soon as $t \neq 0$, $\Psi(t)$ is no more a Slater determinant, while $\Phi(t)$ is confined to be such a determinant. Since anyhow Eq.(1) cannot be solved, the question is, can $\Phi(t)$, given by the solvable Eq.(2), retain some properties of $\Psi(t)$? In particular, can one make a handy theory of nuclear reactions with $\Phi(t)$?

The answer is probably "no". Not just because $\mathcal{U}(\Phi)$ does not account fully for the multiple collision mechanisms implied by $\mathcal{V}$. But also, and maybe mainly, because the behaviour of $\Phi(t)$, when $|t| \to \infty$, is physically too much away from that of $\Psi(t)$.

In the initial work of Bonche et al.[1], as well as in the recent and more developed T.D.H.F. calculations, Φ_o is based on the static Hartree-Fock solutions which describe (approximately) the ground states of the projectile and the target. These static determinants are kicked into translational motion by suitable *phase* excitations. It is then easy to show[1] that, as long as the collision has not started, $\Phi(t)$ describes the translation of target and projectile with respect to each other. *In particular there is no spreading* when $t \to -\infty$, while it is known that $\Psi(t)$, the Schrödinger solution, cannot remain as confined as Φ_o (whether $t \to -\infty$ or $t \to +\infty$).

In order to realize what this difference in spreading behaviour between T.D.S.E. and T.D.H.F. means, let us consider a numerical example[2]. Typically, for a $^{40}Ca - ^{40}Ca$ collision, the T.D.H.F. wave packet for relative motion may have a width λ of order 0.5 fm . If at time $t = 0$ the distance between target and projectile is, say, $\sigma = 10$ fm , one gets an angle uncertainty of order $\Delta\phi \simeq \lambda/\sigma = 1/20$. The orbital momentum fluctuation is then $\Delta\ell \simeq 1/\Delta\phi = 20$, already quite a big number. Now, at an earlier time, one may take, for instance, $\sigma = 20$ fm . Since λ does not change in T.D.H.F. when $t \to -\infty$, $\Delta\phi \simeq 1/40$ and $\Delta\ell \simeq 40$ for that earlier time. It is hard, clearly, to identify such a T.D.H.F. solution with a safe average on partial waves. On the contrary, the spreading of the T.D.S.E. solution allows conservation of the angular momentum width. For instance, if $\sigma = 20$ fm then λ *must* become of order 1 fm for Ψ and thus $\Delta\ell$ remains equal to 20.

It is now clear that something must be done to restore the possibility of an expansion into partial waves. But there is an even more important problem to solve. When $t \to +\infty$, $\Psi(t)$ can be expanded into channels and *the probability of each channel in $\Psi(t)$ becomes a constant*. This is what allows the definition of cross-sections. Unfortunately it seems, however, that one cannot[1] define a similar asymptotic, constant set of channel probabilities in an expansion of $\Phi(t)$.

It looks as if T.D.H.F. is not capable to define anything but gross averages of cross-sections. The solution is then to attempt to relate T.D.H.F. to more traditional theories of nuclear reactions.

Such traditional theories are usually formulated in terms of a time-independent, stationary scattering state $\Psi_{\underset{\sim}{k}}^{(+)}$, with suitable outgoing and ingoing fluxes and asymptotic momentum. What we can try is to reconstruct a $\Psi_{\underset{\sim}{k}}^{(+)}$ on the basis of $\Phi(t)$.

There are several steps in this reconstruction. Technical details can be found in ref.2). The main ideas are the following :

1) First, project $\Phi(t)$ on good angular momentum. Since it is a Slater determinant, such a projection should not be too difficult. One obtains $\Phi_{\ell m}(t) = P_{\ell m}\, \Phi(t)$.

2) Then calculate the Hamiltonian and overlap kernels

$$H_{\ell m}(t,t') = \langle \Phi(t) \,|\, \mathcal{H}\, P_{\ell m} \,|\, \Phi(t') \rangle \quad , \tag{3a}$$

$$N_{\ell m}(t,t') = \langle \Phi(t) \,|\, P_{\ell m} \,|\, \Phi(t') \rangle \quad . \tag{3b}$$

The techniques for such calculations are also standard.

3) Use time as a generator coordinate, by solving the Griffin-Hill-Wheeler equation

$$\int_{-\infty}^{+\infty} dt' \left[H_{\ell m}(t,t') - E\, N_{\ell m}(t,t') \right] f_{\ell m}(t') = 0 \quad , \tag{4}$$

It can be shown[2] that an asymptotic solution of Eq.(4) when $t \to -\infty$ is

$$f_{\ell m}(t) \propto t^{\alpha} \exp(-iEt) \quad , \tag{5}$$

where t^{α} compensates for the lack of spreading and α may depend on m . The function

$$\Psi_{\ell m} = \int_{-\infty}^{+\infty} dt \; f_{\ell m}(t) \; \Phi_{\ell m}(t) \quad , \tag{6}$$

then turns out to be a completely healthy, stationary partial wave.

4) Finally there exists suitable coefficients $c_{\ell m}$ such that

$$\Psi_k^{(+)} = \sum_{\ell m} c_{\ell m} \; \Psi_{\ell m} \quad , \tag{7}$$

is the desired scattering wave of traditional type, to be plugged into any standard formula such as the calculation of a T-matrix element.

To summarize, we have converted $\Phi(t)$, which depends on the continuous label t , into a time-independent state, which is more suitable for the calculation of cross-sections and the partial wave analysis of the nuclear collision.

2. BREAKDOWN AND CURE OF CONSTRAINED HARTREE-FOCK.

The estimation of collective potentials, fission barriers and other energy surfaces by means of C.H.F. calculations is one of the oldest microscopic tool used in nuclear physics. Let $\mathcal{R}$ be, for instance, the quadrupole moment operator. It is customary to claim that one may solve the equation :

$$\delta \langle \Phi | \mathcal{H} - \Lambda \mathcal{R} | \Phi \rangle = 0 \quad , \tag{8}$$

where Λ is a Lagrange multiplier and Φ a normalized trial wave function, usually a Slater determinant. The (expected) lowest solution Φ_Λ of Eq.(8) yields

$$r = \langle \Phi_\Lambda | \mathcal{R} | \Phi_\Lambda \rangle \quad , \tag{9.a}$$

$$e = \langle \Phi_\Lambda | \mathcal{H} | \Phi_\Lambda \rangle \quad , \tag{9.b}$$

and it is often fashionable to refer to e(r) as "the energy surface" or "the real part of the collective potential for quadrupole vibration" et tutti quanti. As pointed out by Fonte and Schiffrer[3] and by Bassichis et al.[4], there is, however, a slight difficulty in generating e(r) without ambiguity.

The point is, e(r) *is just flat* and equal to the ground state energy (or Hartree Fock ground state energy) e_o of $\mathcal{H}$. The proof goes as follows. Let Φ_o be the ground state (or H.F.g.s.) of $\mathcal{H}$. It describes a drop of nuclear matter which is confined within the nuclear radius, except for slight tail effects. Now let Φ_1 be a normalized wave function, with the following properties :

1) The nuclear matter described by Φ_1 must lie far away enough from that of Φ_o , so that off-diagonal matrix elements $\langle \Phi_o | \mathcal{H} | \Phi_1 \rangle$ and $\langle \Phi_o | \mathcal{R} | \Phi_1 \rangle$ are negligibly small ;

2) Φ_1 should be so diffuse that it would carry negligibly small amounts of kinetic and potential energies, $\langle \Phi_1 | \mathcal{H} | \Phi_1 \rangle \approx 0$;

3) Φ_1 should be far enough and deformed enough so that $\langle \Phi_1 | \mathcal{R} | \Phi_1 \rangle$ be enormous.

A good image for Φ_1 is that of an elongated Saturn ring with Φ_o as the planet. It is now obvious that a slight mixture of Φ_1 into Φ_o can make the quadrupole moment arbitray without changing the energy. As a consequence of this "Saturn ring paradox", $e(r) \approx e_o$ whatever r . It looks as if C.H.F. is in a complete breakdown..

One may notice, however, that the second condition above, namely the diffuseness of Φ_1 , has an important effect upon the fluctuation

$$\Delta r_1 = \left[\langle \Phi_1 | \mathcal{R}^2 | \Phi_1 \rangle - \langle \Phi_1 | \mathcal{R} | \Phi_1 \rangle^2 \right]^{1/2} , \qquad (10)$$

because $\mathcal{R}$ is a local operator, the eigenstates of which are certainly not diffuse. Thus Δr_1 is enormous, and small admixtures of Φ_1 into Φ_0 may greatly increase the fluctuation Δr with respect to its initial value Δr_0 taken from Φ_0 .

It seems preferable not to let the collective coordinate $\mathcal{R}$ fluctuate arbitrarily in the study of the energy surface. The constrained Hamiltonian to be considered now appears to become

$$\mathcal{H}' = \mathcal{H} - \Lambda \mathcal{R} + M\mathcal{R}^2 , \qquad (11)$$

with a positive, additional Lagrange multiplier M . It is reasonable to estimate that suitable values of M will reduce the diffuseness of Φ_1 , thus letting Φ_1 carry some energy and that anyhow Δr will diminish. Some structure should reappear in e(r) .

To summarize this section, it makes no sense in designing a microscopic description of a collective coordinate without control of the fluctuation of that coordinate.

3. T.D.H.F., Born-Oppenheimer A.L., G.C.M.

Whether one uses an optical potential to simplify the description of absorption or one labels a whole band of bound states or resonances as a vibration or rotation band, there is some experimental evidence that the nuclear dynamics can sometimes be reduced to a very small set of degrees of freedom. This is fortunate, for indeed a major problem of nuclear theory is to reduce the number of degrees of freedom to be considered, because there are too many variables in $\mathcal{H}$.

There is a well known case in which this reduction can be achieved. It is the Born-Oppenheimer approximation (B.O.A.) in atomic physics. Let $\mathcal{R}$ label the set of "heavy" coordinates (proton or atomic nuclei) and $\mathcal{S}$ label the "light" coordinates. The physical idea behind the method is that, as long as the expectation values of the heavy coordinates describe a motion which is slow enough, then the physical state of the light coordinates

is just *locked* to those expectation values $\langle \mathcal{R} \rangle$.

More precisely, let us split $\mathcal{H}$ into

$$\mathcal{H} = \mathcal{H}_{\mathcal{R}} + \mathcal{V}(\mathcal{R},\mathcal{S}) + \mathcal{H}_{\mathcal{S}} \quad , \tag{12}$$

where $\mathcal{H}_{\mathcal{R}}$ contains only $\mathcal{R}$ and the corresponding momenta, $\mathcal{H}_{\mathcal{S}}$ contains only $\mathcal{S}$ and the corresponding momenta and $\mathcal{V}(\mathcal{R},\mathcal{S})$ is a *local* coupling. The B.O.A. consists

1) in setting $\mathcal{R}$ strictly equal to r and look for the (normalized) solution of the "light equation"

$$\left[\mathcal{V}(r,\mathcal{S}) + \mathcal{H}_{\mathcal{S}} - \varepsilon(r)\right] \chi_r(\mathcal{S}) = 0 \quad , \tag{13}$$

a diagonalization problem in the $\mathcal{S}$ space,

2) then solving the "heavy equation", in $\mathcal{R}$ space,

$$\left[\mathcal{H}_{\mathcal{R}} + \varepsilon(\mathcal{R}) - E\right] \xi(\mathcal{R}) = 0 \quad , \tag{14}$$

3) and finally claiming that

$$\Psi(\mathcal{R},\mathcal{S}) = \xi(\mathcal{R})\, \chi_{\mathcal{R}}(\mathcal{S}) \tag{15}$$

is a reasonable eigenstate of $\mathcal{H}$.

We shall now write Eqs.(13) to (15) in a different way. First, we notice that $\chi_r(\mathcal{S})$ can be associated to a state $\phi_r(\mathcal{R},\mathcal{S}) = \delta(\mathcal{R} - r)\, \chi_r(\mathcal{S})$ which now belongs to the full Hilbert space of both $\mathcal{R}$ and $\mathcal{S}$. Thus Eq.(13) is identical to the constrained variational problem

$$\delta \langle \phi | \mathcal{H} | \phi \rangle_r = 0 \quad , \tag{13.a}$$

the constraint being that $\langle \mathcal{R} \rangle$ should be equal to r , without any fluctuation. (Actually, because of this lack of tolerance for fluctuation, Eq.(13.a) is singular, because the δ-function contained in ϕ_r makes trouble with the kinetic energy contained in $\mathcal{H}_{\mathcal{R}}$. But it is clear that this divergence can be removed if one accepts a finite width wave packet $\Gamma(\mathcal{R} - r)$ in ϕ_r rather than the sharp δ-function. This question will be met again below).

Now Eq.(15) also reads :

$$\Psi(\mathcal{R},\mathcal{S}) = \int dr\ \xi(r)\ \delta(\mathcal{R}-r)\ \ \chi_r(\mathcal{S})$$
$$= \int dr\ \xi(r)\ \Phi_r(\mathcal{R},\mathcal{S}) \quad , \qquad (15.a)$$

which is already a R.G.M. or G.C.M. representation of the Born-Oppenheimer ansatz. We have only to show now that Eq.(14) amounts to a Griffin-Hill-Wheeler (G.H.W.) equation. This goes as follows.

For the sake of simplicity, let $\mathcal{H}_{\mathcal{R}}$ be a sum of local potentials $\mathcal{V}(\mathcal{R})$ and kinetic energy Laplacians $-\Delta_{\mathcal{R}}$. If one takes Φ_r as a generating function, the G.H.W. equation reads

$$\int dr\ \langle \delta(r'-\mathcal{R})\ \chi_{r'} \mid \mathcal{H}_{\mathcal{R}} + \mathcal{V}(\mathcal{R},\mathcal{S}) + \mathcal{H}_{\mathcal{S}} - E \mid \delta(r-\mathcal{R})\ \chi_r \rangle\ f(r) = 0 \ . \qquad (14.a)$$

Because of Eq.(13), and because $\langle \Phi_{r'} \mid \Phi_r \rangle = \delta(r-r')$, this becomes

$$\langle \delta(r'-\mathcal{R})\chi_{r'} \mid -\Delta_{\mathcal{R}} \mid f(\mathcal{R})\ \chi_{\mathcal{R}} \rangle + \left[\mathcal{V}(r') + \varepsilon(r') - E\right]\ f(r') = 0 \qquad (14.b)$$

The B.O.A. consists in letting the Laplacians act upon f only. One neglects the derivatives of $\chi_{\mathcal{R}}$ with respect to $\mathcal{R}$. Then Eq.(14.b) can be simplified by letting the last integral upon $\mathcal{S}$ be performed in the bracket, and one obtains

$$\left[-\Delta_{r'} + \mathcal{V}(r') + \varepsilon(r') - E\right]\ f(r') = 0 \quad , \qquad (14.c)$$

which is nothing but Eq.(14) with different notations. It can be stressed at that point that, because of Eq.(14.a), the left-hand side operator of Eq.(14) is equal to the projection of $\mathcal{H}$ into the subspace spanned by Φ_r : The only difference is the fact that we have neglected derivatives of χ_r .

The scheme to be used in nuclear physics is now easy to guess :

1) Generate a set of generator functions ϕ_r , square integrable functions depending on both $\mathcal{S}$ and $\mathcal{R}$, with the constraint $\langle \phi_r \mid \mathcal{R} \mid \phi_r \rangle = r$ and a small (but finite, in order to avoid singularities) width. They are solutions of

$$\delta \langle \varphi \mid \mathcal{H} - \Lambda \mathcal{R} + M\mathcal{R}^2 \mid \phi \rangle = 0 \qquad (13.b)$$

2) Calculate the coordinate and overlap kernels

$$\begin{Bmatrix} R(r,r') \\ N(r,r') \end{Bmatrix} = \langle \phi_r | \begin{Bmatrix} \mathcal{R} \\ 1 \end{Bmatrix} | \phi_{r'} \rangle \qquad (16)$$

and solve the generator coordinate problem for $\mathcal{R}$ (not for $\mathcal{H}$, yet !)

$$\int dr \; [R(r',r) - \rho \, N(r',r)] \; a(r) = 0 \qquad (17)$$

The functions

$$\phi_\rho = \int dr \; a(r) \; \phi_r \qquad (18)$$

fulfill the conditions $\langle \phi_\rho | \phi_{\rho'} \rangle = \delta(\rho-\rho')$ and $\langle \phi_\rho | \mathcal{R} | \phi_{\rho'} \rangle = \rho \, \delta(\rho-\rho')$. In other words, they define the basis of the generator subspace which makes $\mathcal{R}$ a c-number. To a good approximation, therefore

$$\phi_\rho(\mathcal{R}, \mathcal{Y}) = \delta(\mathcal{R} - \rho) \; \chi_\rho(\mathcal{Y}) \qquad (15.b)$$

3) The dynamical equation to solve is

$$\int d\rho \; [\langle \phi_{\rho'} | \mathcal{H} | \phi_\rho \rangle - E] \quad \xi(\rho) = 0 \quad , \qquad (14.d)$$

which shows that the collective Hamiltonian is only the representation of $\mathcal{H}$ on a basis which makes $\mathcal{R}$ a c number.

Nothing prevents to attempt a parametrization of that collective Hamiltonian $\langle \phi_{\rho'} | \mathcal{H} | \phi_\rho \rangle$ in terms of an effective mass and a potential. More details can be found elsewhere[6]. Analytical and numerical results[6] have been used as a check of the above prescriptions *1)* to *3)*. For the time being, there seems to be no flagrant inconsistency in these prescriptions, as checked by these numerical results.

It must be noticed that Eq.(14.d) takes into account the derivatives of χ_ρ which were neglected in Eq.(14.c). This means that $\langle \phi_\rho | \mathcal{H} | \phi_\rho \rangle$ may contain some non-local potential. Let $\overline{W}(\rho,\rho')$ be that potential. If one wants only local potentials and effective masses, one must expand $\overline{W}$ in terms like $\delta(\rho-\rho')$, $\delta''(\rho-\rho')$ and so on (actually one usually stops at second order). The bare mass m_o will become a renormalized mass[6] m given

by :

$$m^{-1} = m_o^{-1} - \int (\rho-\rho')^2 \, \overline{W}(\rho,\rho') \, d(\rho-\rho') \qquad (19)$$

If $\overline{W}(\rho,\rho')$ is always positive and large enough, then m^{-1} may become negative. We thus find an interesting criterion for the validity of the formalism : a negative mass is an indication of too strongly repulsive a *non-local* interaction. The B.O.A., which is based on a low velocity dependence for $\mathcal{R}$, then becomes suspect.

To summarize this section, the adiabatic limit permits a unification of the constrained Hartree-Fock method, the Born-Oppenheimer approximation and the generator coordinate method. There is, however, an important preliminary step, namely the guess of $\mathcal{R}$. It may be that the adiabatic time-dependent Hartree-Fock theory[7] can give a way to select $\mathcal{R}$ properly.

4. FINAL REMARKS ON CONTINUITY

For large amplitude nuclear motions, a time dependent description probably makes little difference between a bound oscillation and one that leads to break-up of the nucleus. It is only a matter of going over specific thresholds. Now, in the asymptotic regions, the collective degree of freedom are well known : they are just the distance coordinates in the various channels. The collective masses are bare reduced masses and one has also reasonable estimates of the corresponding potentials. It is therefore reasonable to expect that, if there is a path which describes as well, say, quadrupole oscillations of small than those of large amplitude, the quadrupole mass and potential should be continuous functions along the path and finally become simply related to the bare mass and potential of the corresponding fission mode.

At higher energies, when a B.O.A. is not valid, because the degrees of freedom $\mathcal{S}$ are not locked any more to $\mathcal{R}$, it might still happen that the influence of $\mathcal{S}$ averages only into a loss of energy for $\mathcal{R}$. The *statistical* average path might still be *stable.* If that delicate problem of stability can be properly formulated in a statistical theory, then again one may expect some continuity between the channel region and the interaction region. A study of the stability (on the average) of T.D.H.F.

evolution with respect to some randomness of initial conditions is then in order.

To conclude this report, it can be said that the continuous basis of Slater determinants provided either by T.D.H.F. or by C.H.F. appears like a very useful first step, the second step being to perform a generator coordinate calculation upon that basis.

Most of the work reported here has been done with B. Grammaticos and J. Le Tourneux. It is a pleasure to thank the organisors of this Symposium for their hospitality and the opportunity of giving this report.

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DISCUSSION

H. Hofmann: You showed in the second part of your talk a dramatic change of the shape of the potential landscape with increasing the basis. It seems to me that no final inference can be drawn from this fact if the kinetic energy is not computed at the same time. After all it is this kinetic energy which defines the metric for these collective degrees. Would you agree on that?

B.G.Giraud: I certainly agree that one should also look at the behaviour of the collective mass. Still, our classical intuition tells us that the flat energy surface is an unpleasant phenomenon and it looks desirable to maintain the fluctuation of the collective coordinate within reasonable finite values.