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**BORN-OPPENHEIMER COUPLING BETWEEN COLLECTIVE AND
INTRINSIC DEGREES OF FREEDOM**

by

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Abstract :

The splitting of the nuclear Hamiltonian into a collective Hamiltonian, an intrinsic Hamiltonian and a coupling term is shown to be a solvable problem. The solution is equivalent to a change of representation, as exemplified by the multi-channel theory of nuclear scattering or the Born-Oppenheimer representation of molecular dynamics.

Most nuclear models¹⁾ attempt to replace the microscopic description of N nucleons, with their $3N$ degrees of freedom ξ_1, \dots, ξ_N and corresponding Hamiltonian $\mathcal{H}(\xi_1, \dots, \xi_N, \mathcal{R}_1, \dots, \mathcal{R}_N)$, by a description with much fewer degrees of freedom $\mathcal{R}_1, \dots, \mathcal{R}_C$, $C \ll 3N$. The variables \mathcal{R} are understood to be "collective" and governed by a collective Hamiltonian $\mathcal{H}_{\text{coll}}(\mathcal{R}_1, \dots, \mathcal{R}_C, \mathcal{P}_1, \dots, \mathcal{P}_C)$. As regards the connection between \mathcal{R}'_s and ξ 's and the derivation of $\mathcal{H}_{\text{coll}}$ from \mathcal{H} , a certain amount of arbitrariness and phenomenology in the choice of \mathcal{R}'_s and properties of $\mathcal{H}_{\text{coll}}$ is unavoidable, if only because there exist $3N-C$ residual degrees of freedom ξ_1, \dots, ξ_{3N-C} . An explicit change of coordinates from ξ 's into \mathcal{R} 's and ξ 's is usually impossible. The purpose of this note is to show, however, that the problem is not untractable.

The main question to be raised is how to estimate the coupling between the "intrinsic" degrees of freedom ξ and the collective variables \mathcal{R} . For this coupling may induce important viscosity and/or friction effects in the collective dynamics, as is well known in the

theory of the deep inelastic collisions of heavy ions for instance. There one chooses for \mathcal{R} 's the relative distance between the ions and a few other variables such as deformation parameters, angular momenta or orientation angles of fragments in binary modes, mass and charge densities and so on²⁾. The influence of the neglected intrinsic degrees of freedom is then felt through an interesting hierarchy of relaxation times for the \mathcal{R} 's.

A similar question is of importance in the theory of fission³⁾, since the statistical distribution in the phase space of \mathcal{R} 's is actually controlled by the ξ 's. For instance the mass distribution of final products, a collective observable, may be influenced by the presence or absence of the breaking of pairing between nucleons, an intrinsic mechanism⁴⁾. Many other examples can be found where the coupling between \mathcal{R} 's and ξ 's needs to be properly understood⁵⁾.

The argument which now follows goes by three steps. It will first be stressed that the theory of coupled channels in nuclear collisions actually achieves a change of variables from \underline{r} 's to \mathcal{R} 's and ξ 's, in a special representation⁶⁾, though. Then it will be shown that the formalism can be extended to a Born-Oppenheimer representation⁷⁾ for coupled channels. Finally the general situation, where approximations can be implemented in a practical way, will be described.

In the theory of coupled channels one knows explicitly the 6 collective variables, namely the total center-of-mass coordinate vector $\underline{R} = (\underline{r}_1 + \dots + \underline{r}_N)/N$ and the relative distance vector $\underline{\mathcal{R}}$ between the projectile A and target B

$$\underline{\mathcal{R}} = (\underline{r}_1 + \dots + \underline{r}_A)/A - (\underline{r}_{A+1} + \dots + \underline{r}_{A+B})/B \quad (1)$$

The 3N-6 intrinsic variables are the internal Jacobi coordinates of nuclei A and B, such as

$$\begin{aligned} \xi_1 &= \tilde{r}_1 - \tilde{r}_2, & \xi_2 &= \tilde{r}_3 - (\tilde{r}_1 + \tilde{r}_2)/2, \dots \\ \xi_{A-1} &= \tilde{r}_A - (\tilde{r}_1 + \dots + \tilde{r}_{A-1})/(A-1), & \xi_A &= \tilde{r}_{A+1} - \tilde{r}_{A+2}, \dots \end{aligned} \quad (2)$$

$$\xi_{A+B-2} = \tilde{r}_{A+B} - (\tilde{r}_{A+1} + \dots + \tilde{r}_{A+B-1})/(B-1) .$$

As the transformation from \tilde{r} 's to \mathcal{R} 's and ξ 's is here linear, it is a priori possible in the cluster model and the associated resonating group method⁸⁾ to transform explicitly the nuclear Hamiltonian from its microscopic representation

$$\mathcal{H} = \sum_{i=1}^{N=A+B} \frac{p_i^2}{2m} + \sum_{i>j=1}^N V(\tilde{r}_i - \tilde{r}_j) \quad (3)$$

into the partition representation

$$\mathcal{H} = \mathcal{H}_{\text{coll}} + \mathcal{H}_{\text{int}} + \mathcal{H}_{\text{coupl}} \quad (4)$$

with

$$\mathcal{H}_{\text{coll}} = \frac{P^2}{2Nm} + \frac{\mathcal{P}^2}{2\mu m} \quad (5)$$

$$\begin{aligned} \mathcal{H}_{\text{int}} = \mathcal{H}_A + \mathcal{H}_B &= \left[\sum_{k=1}^{A-1} \frac{\pi_k^2}{2\mu_k m} + \sum_{i>j=1}^A V(\tilde{r}_i - \tilde{r}_j) \right] \\ &+ \left[\sum_{k=A}^{A+B-2} \frac{\pi_k^2}{2\mu_k m} + \sum_{i>j=A+1}^{A+B} V(\tilde{r}_i - \tilde{r}_j) \right] \end{aligned} \quad (6)$$

and

$$\mathcal{H}_{\text{coupl}} = \sum_{i=1}^A \sum_{j=A+1}^{A+B} V(\tilde{r}_i - \tilde{r}_j) \quad (7)$$

In these eqs. (5) to (7) the momenta \underline{P} , \underline{Q} and $\underline{\pi}_k$ are conjugate to \underline{R} , \underline{Q} and $\underline{\xi}_k$, respectively, and they are associated to the relevant masses Nm , $\mu m = \frac{AB}{N} m$ and $\mu_k m$. It is obvious that \mathcal{H}_{coll} , \mathcal{H}_{int} and \mathcal{H}_{coupl} are the collective, intrinsic and coupling Hamiltonians, respectively.

The channel representation consists first in the diagonalization of \mathcal{H}_{int} , with eigenfunctions $\chi_n(\underline{\xi})$ which are products of eigenstate of nuclei A and B,

$$\chi_n(\underline{\xi}) = \chi_{n_A}(\xi_1 \dots \xi_{A-1}) \chi_{n_B}(\xi_A \dots \xi_{A+B-2}) \quad , \quad (8)$$

$$\mathcal{H}_{int} \chi_n = (\epsilon_{n_A} + \epsilon_{n_B}) \chi_n \quad , \quad (9)$$

the eigenvalue ϵ_n being obviously the sum of nuclear eigenenergies.

Then a complete basis of the full Hilbert space of the $3N$ degrees of freedom may be chosen as

$$\phi_{\underline{R}', \underline{Q}', n}(\underline{R}, \underline{Q}, \underline{\xi}) = \delta(\underline{R} - \underline{R}') \delta(\underline{Q} - \underline{Q}') \chi_n(\underline{\xi}) \quad , \quad (10)$$

where \underline{R}' and \underline{Q}' are c-numbers taking on all values.

Except for details of antisymmetrization which are unnecessary in the present discussion, this is nothing but the basis of the resonating group method⁸⁾. In this representation the general, non diagonal matrix element of \mathcal{H} reads

$$\begin{aligned} \langle \phi_{\underline{R}', \underline{Q}', n'} | \mathcal{H} | \phi_{\underline{R}'', \underline{Q}'', n''} \rangle &= -\delta_{n', n''} \left[\frac{\Delta_{\underline{R}''}}{2Nm} + \frac{\Delta_{\underline{Q}''}}{2\mu m} \right] \delta(\underline{R}' - \underline{R}'') \delta(\underline{Q}' - \underline{Q}'') \\ &+ \delta(\underline{R}' - \underline{R}'') \delta(\underline{Q}' - \underline{Q}'') \epsilon_n \delta_{n', n''} + \langle \phi_{\underline{R}', \underline{Q}', n'} | \mathcal{H}_{coupl} | \phi_{\underline{R}'', \underline{Q}'', n''} \rangle \quad . \end{aligned} \quad (11)$$

It will be noticed here that the first term in the right-hand-side of eq. (11) is diagonal with respect to the intrinsic labels n', n'' and corresponds to the collective Hamiltonian. The second term is diagonal

with respect to the collective labels \underline{R}' , \underline{R}' , \underline{R}'' , \underline{R}'' and corresponds to the internal Hamiltonian. The last term has no a priori diagonal properties and is identified as the interaction matrix element. This classification will be of some use in the following. The diagonalization of \mathcal{H} in this representation, eq. (11), is nothing but the coupled channel theory of scattering, the details of which are well known and need not be recalled. Truncations on the channel labels n are, obviously, the most natural approximations available for practical calculations.

The Born-Oppenheimer representation shows similar properties. As will be shown, however, the presence in the formalism of adiabatic polarization effects induces a modification in the three terms which will be found in the right-hand side of an equation analogous to eq. (11). Let \underline{R} denote all the "heavy" degrees of freedom (protons, nuclei) and $\underline{\xi}$ denote the "light" degrees of freedom (electrons). Again the Hamiltonian is the sum of three terms

$$\mathcal{H} = \mathcal{H}_{\text{heavy}}(\underline{R}) + \mathcal{H}_{\text{light}}(\underline{\xi}) + \mathcal{V}(\underline{R}, \underline{\xi}) \quad , \quad (12)$$

but these terms will not be interpreted like those of eq. (4). Rather, taking advantage of the fact that \mathcal{V} is a local operator with respect to \underline{R} , one replaces eq. (9) by a diagonalisation of $\mathcal{H}_{\text{light}} + \mathcal{V}$ in the full Hilbert space of both \underline{R} and $\underline{\xi}$,

$$[\mathcal{H}_{\text{light}}(\underline{\xi}) + \mathcal{V}(\underline{R}, \underline{\xi}) - \epsilon_n(\underline{R}')]\phi_{\underline{R}', n} = 0 \quad , \quad (13)$$

where

$$\phi_{\underline{R}', n}(\underline{R}, \underline{\xi}) = \delta(\underline{R} - \underline{R}') \chi_{\underline{R}', n}(\underline{\xi}) \quad , \quad (14)$$

with again \underline{R}' as a c-number. Comparison with eq. (10) shows that χ is now again a channel wave function, with \underline{R}' -dependent polarization

effects however.

The functions $\phi_{\mathcal{R}'n}$ make a complete, orthonormal basis of the full Hilbert space, for obviously

$$\langle \phi_{\mathcal{R}'n} | \phi_{\mathcal{R}''n} \rangle = \delta(\mathcal{R}' - \mathcal{R}'') \delta_{n'n''} \quad (15)$$

because of the hermiticity of $\mathcal{H}_{\text{light}} + \mathcal{V}$ and because of eqs. (13) and (14). For the same reasons one finds the completeness relation

$$\begin{aligned} \sum_n \int d\mathcal{R}' \chi_{\mathcal{R}'n}^*(\xi_1) \delta(\mathcal{R}_1 - \mathcal{R}') \delta(\mathcal{R}_2 - \mathcal{R}') \chi_{\mathcal{R}'n}(\xi_2) \\ = \sum_n \chi_{\mathcal{R}'n}^*(\xi_1) \delta(\mathcal{R}_1 - \mathcal{R}_2) \chi_{\mathcal{R}'n}(\xi_2) \\ = \delta(\mathcal{R}_1 - \mathcal{R}_2) \delta(\xi_1 - \xi_2) \end{aligned} \quad (16)$$

It is now interesting to consider the matrix element of \mathcal{H} in this representation. One finds at once, from eqs. (12) to (14),

$$\begin{aligned} \langle \phi_{\mathcal{R}'n} | \mathcal{H} | \phi_{\mathcal{R}''n} \rangle = \langle \phi_{\mathcal{R}'n} | (\mathcal{T} + \mathcal{U}) | \phi_{\mathcal{R}''n} \rangle \\ + \delta(\mathcal{R}' - \mathcal{R}'') \epsilon_n(\mathcal{R}') \delta_{n'n''} \end{aligned} \quad (17)$$

where it is necessary to distinguish the kinetic and potential parts,

\mathcal{T} and \mathcal{U} , respectively, which are present in $\mathcal{H}_{\text{heavy}}$. For a local operator $\mathcal{U}(\mathcal{R})$ gives a term diagonal with respect to \mathcal{R} while \mathcal{T} , which contains Laplacians, induces three terms. More precisely, since $\phi_{\mathcal{R}'n}$, eq. (14), is the product of a δ -function and an \mathcal{R}' dependent intrinsic state, it is well known that the gradient operator may act twice on either the former or the latter, and it may also act once on each.

If one denotes by $M_{\beta\gamma}$ the mass tensor which defines \mathcal{T} and assumes

that this mass tensor is a constant, one finds

$$\begin{aligned}
 \langle \phi_{\mathcal{R}'n'} | \mathcal{H} | \phi_{\mathcal{R}''n''} \rangle = & \delta_{n'n''} \left[\sum_{\beta, \gamma=1}^C \frac{\partial}{\partial \mathcal{R}''_{\beta}} \frac{1}{2M_{\beta\gamma}} \frac{\partial}{\partial \mathcal{R}''_{\gamma}} \delta(\mathcal{R}' - \mathcal{R}'') \right. \\
 & + \mathcal{U}(\mathcal{R}') \delta(\mathcal{R}' - \mathcal{R}'') \left. \right] + \delta(\mathcal{R}' - \mathcal{R}'') \epsilon_{n'}(\mathcal{R}') \delta_{n'n''} \\
 & - \sum_{\beta, \gamma=1}^C \left[W_{n'n''}^{\beta\gamma}(\mathcal{R}'') + W_{n'n''}^{\beta}(\mathcal{R}'') \frac{\partial}{\partial \mathcal{R}''_{\gamma}} + \frac{\partial}{\partial \mathcal{R}''_{\beta}} W_{n'n''}^{\gamma}(\mathcal{R}'') \right] \delta(\mathcal{R}' - \mathcal{R}'')
 \end{aligned} \tag{18}$$

where

$$W_{n'n''}^{\beta\gamma}(\mathcal{R}'') = \frac{1}{2M_{\beta\gamma}} \int d\xi \chi_{\mathcal{R}''n''}^*(\xi) \frac{\partial^2}{\partial \mathcal{R}''_{\beta} \partial \mathcal{R}''_{\gamma}} \chi_{\mathcal{R}''n''}(\xi), \tag{19}$$

and

$$W_{n'n''}^{\beta}(\mathcal{R}'') = \frac{1}{2M_{\beta\gamma}} \int d\xi \chi_{\mathcal{R}''n''}^*(\xi) \frac{\partial}{\partial \mathcal{R}''_{\beta}} \chi_{\mathcal{R}''n''}(\xi). \tag{20}$$

The first bracket (a sum of two terms) in the right hand side of eq. (18) may at first sight be understood as the collective Hamiltonian. It is actually renormalized by the intrinsic Hamiltonian driven by \mathcal{U} , $\epsilon_{n'}(\mathcal{R}') \delta_{n'n''} \delta(\mathcal{R}' - \mathcal{R}'')$. The last bracket in the r.h.s. of eq. (18) has, obviously, the structure of a coupling term between channels. It is a sum of two terms, one with local form factors $W^{\beta\gamma}$ and one with quasi-local form factors W^{β} . The properties of the Born-Oppenheimer multi-channel theory results from multiplying the ansatz

$$\Psi(\mathcal{R}, \xi) = \sum_{n''} \int d\mathcal{R}'' \mathcal{E}_{n''}(\mathcal{R}'') \phi_{\mathcal{R}''n''} \tag{21}$$

where $\phi_{\mathcal{R}''n''}$ has been defined by eq. (14), by the total Hamiltonian \mathcal{H} as described by eq. (18). When solving at best the Schrödinger equation one may truncate with respect to the channel indices $n'n''$, thus obtaining a canonical system of coupled differential equations for

the unknown wave function g_n .

It can be stressed at this point of the argument that the "channel" index n defines an intrinsic representation more convenient than the "intrinsic coordinate representation" ξ . This is because the change of representation from $\{\mathcal{R}, \xi\}$ to $\{\mathcal{R}, n\}$ defines the channel basis $\phi_{\mathcal{R}n}$, the physical significance of which is obvious. It will now be shown that a more general case can be found where coupling terms $W_{n'n}$ can be exhibited.

The procedure goes as follows. Let \mathcal{R} be a set of microscopic nuclear operators (multipole moments, etc) for which there is evidence of collective motion. A constrained Hartree-Fock calculation can then generate a discrete set of Slater determinants $\omega_{\lambda\nu}$, where λ is the Lagrange multiplier and ν a discrete label. When λ takes on all relevant values, this makes a discrete set of continuous sequences and nothing prevents to diagonalize \mathcal{R} in the subspace spanned by either one, or all of these sequence $\{\omega_{\lambda\nu}\}$. Namely, within one sequence, one may look for an amplitude $f_{\mathcal{R}'\nu(\lambda)}$ such as the states

$$\tilde{\phi}_{\mathcal{R}'\nu} = \int d\lambda f_{\mathcal{R}'\nu(\lambda)} \omega_{\lambda\nu} \quad , \quad (22)$$

fulfil the properties

$$\langle \tilde{\phi}_{\mathcal{R}'\nu} | \tilde{\phi}_{\mathcal{R}''\nu} \rangle = \delta(\mathcal{R}' - \mathcal{R}'') \quad , \quad (23)$$

and

$$\langle \tilde{\phi}_{\mathcal{R}'\nu} | \mathcal{R} | \tilde{\phi}_{\mathcal{R}''\nu} \rangle = \mathcal{R}' \delta(\mathcal{R}' - \mathcal{R}'') \quad . \quad (24)$$

If the sequences are mixed by the ansatz

$$\tilde{\phi}_{\mathcal{R}'n} = \sum_{\nu} \int d\lambda f_{\mathcal{R}'\nu(\lambda)}^n \omega_{\lambda\nu} \quad , \quad (25)$$

one looks for the properties

$$\langle \tilde{\phi}_{\mathcal{R}'n} | \tilde{\phi}_{\mathcal{R}''n} \rangle = \delta_{n'n''} \delta(\mathcal{R}' - \mathcal{R}'') \quad (26)$$

$$\langle \tilde{\phi}_{\mathcal{R}'n} | \mathcal{R} | \tilde{\phi}_{\mathcal{R}''n} \rangle = \mathcal{R}' \delta_{n'n''} \delta(\mathcal{R}' - \mathcal{R}'') \quad (27)$$

In any case, eqs. (23-24) or (26-27), the diagonalisation of \mathcal{R} is just a generator coordinate ⁹⁾ problem.

The point of interest is that $\tilde{\phi}_{\mathcal{R}'n}$ appears like a normalized eigenstate of \mathcal{R} . A comparison of eqs. (14) and (15) with eqs. (25) and (26) for instance shows that one may identify, at least qualitatively, $\tilde{\phi}_{\mathcal{R}'n}$, eq. (25), with a Born-Oppenheimer channel state $\phi_{\mathcal{R}'n}$, eq. (14). Nothing then prevents, in principle, to calculate the matrix element $\langle \tilde{\phi}_{\mathcal{R}'n} | \mathcal{H} | \tilde{\phi}_{\mathcal{R}''n} \rangle$ and fit it with a form analogous to eq. (18).

Namely, by least square fits or any other suitable method, one can try to extract from $\langle \tilde{\phi}_{\mathcal{R}'n} | \mathcal{H} | \tilde{\phi}_{\mathcal{R}''n} \rangle$

i) a term proportional to $\delta_{n'n''} \delta(\mathcal{R}' - \mathcal{R}'')$, which will account for a renormalizable, channel potential $\epsilon_n + \mathcal{V}$,

ii) a term proportional to $\delta_{n'n''}$ and second derivatives of $\delta(\mathcal{R}' - \mathcal{R}'')$, which will account for collective kinetic energies and possibly contain effective masses $M_{\beta\gamma}(\mathcal{R}'')$,

iii) a term proportional to $\delta(\mathcal{R}' - \mathcal{R}'')$, but non diagonal with respect to $n'n''$, which will account for $\sum_{\beta\gamma} \mathcal{W}_{n'n''}^{\beta\gamma}$, and finally

iv) terms proportional to $\frac{\partial}{\partial \mathcal{R}_\beta} \delta(\mathcal{R}' - \mathcal{R}'')$, which account for $\mathcal{W}_{n'n''}^\beta$.

Although tedious in practice, this derivation of coupling terms between collective and intrinsic degrees of freedom can be summarized easily. Firstly, one should identify collective degrees of freedom and freeze them in an adiabatic approximation such as the constrained

Hartree-Fock method. Secondly, one should diagonalize these operators in order to obtain a suitable channel representation. Finally, the matrix element of the many-body Hamiltonian can just be analyzed in this representation. The coupling under study is only the non-diagonality of this matrix element with respect to the channel index.

It is remarkable that only two kinds of terms, listed above under iii) and iv), are necessary.

The key point of this derivation is the use, for the intrinsic degrees of freedom, of the "n" label, actually an energy label, rather than the ξ label, for the latter raises an untractable problem of an explicit change of coordinates. The difficulty has been alleviated by the channel representation, which may easily incorporate polarization effects and technical truncations.

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REFERENCES

1) See for instance :

- A. Bohr and B.R. Mottelson, Mat. Fys. Medd. Dan. Vid. Selsk 27, n°16
(1953)
- R. Nix and W. Swiatecki, Nucl. Phys. 71, 1 (1965)
- M. Lefort et C. Ngô, Ann. Phys. 1978 V3, 5
- H. Weidenmüller, Transport theories of heavy ion reactions, to be
published in Progress in particle and nuclear physics, ed. D. Wiltonson
(Pergamon, London), preprint MPI-1978-V29
- H. Hofmann and P.J. Siemens, Nucl. Phys. A257, 165 (1976)
- H. Hofmann et al, IV th Balaton Conference Nucl. Phys. Kesztheley 1979
- D.H.E. Gross, Microscopic and Phenomenological Studies on Nuclear Friction,
preprint HMI-B335.

2) C. Grégoire, H. Hofmann, C. Ngô, XVIII Int. Winter Meeting on Nuclear
Physics, Bormio, 1980

C. Grégoire, C. Ngô, B. Renaud, preprint DPhN/MF 80/28

3) K. Pomorki and H. Hofmann, International Workshop on Cross properties
of nuclei and nuclear excitations VIII, Hirschegg 1980 and to be pu-
blished

M.C. Nemes and H.A. Weidenmüller, preprint MPI H - 1980 - V23

4) S. Amiel and H. Fedstein, Proc. of Int. Symp. of Phys. and Chem. of
fission (Rochester 1974) IAEA Vol. II, 65.

5) In particular see :

D. Bohm and Pines, Phys. Rev. 92, 609 (1953)

- 6) B. Giraud, J. Le Tourneux and E. Osnes, Phys. Rev. C11, 82 (1975)
- 7) B. Giraud, Fyzika 9, Suppl. 3, 345 (1977)
- 8) K. Wildermuth and N. Mc Clure, Cluster Representation of Nuclei,
Springer Verlag, Berlin (1966)
- 9) D.L. Hill and J.A. Wheeler, Phys. Rev. 89, 1102 (1953)
J.J. Griffin and J.A. Wheeler, Phys. Rev. 108, 311 (1957)

