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Review of contribution and discussions at the working seminar, Ljubljana, August 13 - September 9, 1972

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GENERATOR COORDINATE METHOD FOR NUCLEAR BOUND STATES AND REACTIONS

A review edited by M.V.MIHAILOVIĆ and M.ROSINA on the basis of discussions and contributions of some participants

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P R E F A C E

In the period of some great successes of the Projected Hartree-Fock, the Projected Hartree-Bogoljubov and the Alpha-particle Models one is asking the question: what comes next? How to go beyond those schemes, whose difficulties and limitations have become recognized? One of the promising schemes which has been in the air for a long time is the Generator Coordinate Method. This method allows the use of an intuitive picture of the nuclear motion and the possibility to build some relevant physical information (but also some prejudice) into the calculation. In addition to simpler interpretation of results, it requires a smaller basis than its rival-the complete diagonalization in a given single-particle basis. In nuclear reaction, progress has been done with the Resonating Group Theory, but there are serious difficulties how to apply it to heavier nuclei. The Generator Coordinate Method promises to be less restrictive.

So a small group of physicists gathered at a working seminar in Ljubljana to discuss which properties of the Generator Coordinate Method can be considered as well understood and which ones are problematic. Also, this "resonating group" tried to review the few phenomena where the Generator Coordinate Method has been used so far and to see which phenomena could be studied in the near future. The discussions and reviews resulted in writing down this Review which should encourage ourselves and other readers to pursue some promissing problems with the Generator Coordinate Method.

The review of the past and the present attempts is rather incomplete. It does not contain the review of the classical works (Hill, Wheeler and Griffin, Peierls, Yoccoz and Thouless) because it was assumed that these works are well known to the participant of the working seminar. Secondly, at the Generator Coordinate Seminars some topics and aspects only were discussed. We feel that

a more complete historical outline should be added at some later time,giving the appropriate credit to all the pioneers in this field.

The activity of the participants was enhanced by the stimulating friendly atmosphere during the seminar. Important collective modes of the participants were reached also when relaxing from hard work, during the attempts to apply the Generator Coordinate Method to the wave motion of the Adriatic Sea and the lake of Bled and to the scattering state of Plitvice waterfalls. The final collective mode is incorporated in these Proceedings.

There is no conclusion in these Proceedings. The conclusion should be writen later, when the "resonating group" reaches its next resonance somewhere in the polygon Ljubljana-Strassbourg-Saclay-Bordeaux-Coimbra-Oxford-Mol-Jülich-Münster. The working seminar on the Generator Coordinate Method was hopefuly not a single event (just to exchange the news) but an initiative towards a long-term collaboration as long as the Generator Coordinate Method is productive.

The Institute "J.Stefan" and the Faculty of Natural Sciences and Technology would like to thank the guests for their active participation to the work of the seminar. The participants exchanged ideas, they explained to each other the work in progress and they planned the future work; they also exchanged programs. So a lot of parallel work in the future will be avoided. They discussed also the differences in the approaches to the work in Ljubljana and in their institutions. So this Seminar was not only a rather new approach to the solving physics problems, but contributed also to the sharing of common knowledge.

Ljubljana, March 15, 1973

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CONTENTS

1. INTRODUCTION

In the Generator Coordinate Method (GCM) [1] one considers a family of N-particle functions $\Phi(x,\alpha)$ where x denotes all particle coordinates, and α stands for a set of m parameters $\alpha_1, \ldots \alpha_m$. With the help of the generator functions $\Phi(x,\alpha)$ approximate eigenfunctions of the N-particle systems are generated by taking linear combinations

$$\Psi(x) = \int f(\alpha)\, \Phi(x,\alpha) d\alpha \ . \qquad (1.1)$$

Here the integration is performed over the m-dimensional space of parameters $\alpha_1, \ldots \alpha_m$. The amplitude function $f(\alpha)$ is determined from the variation principle

$$\delta(\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle) = 0 \ , \qquad (1.2)$$

where H is the Hamiltonian of the system. Eq. (1.2) leads to an integral equation for $f(\alpha)$

$$\int \{H(\alpha',\alpha) - EI(\alpha',\alpha)\}\, f(\alpha) d\alpha = 0 \ , \qquad (1.3)$$

where the kernels $H(\alpha',\alpha)$ and $I(\alpha',\alpha)$ are

$$H(\alpha',\alpha) = \langle\Phi(x,\alpha')|H|\Phi(x,\alpha)\rangle$$

$$I(\alpha',\alpha) = \langle\Phi(x,\alpha')|\Phi(x,\alpha)\rangle \qquad (1.4)$$

The set of states $\Psi(x)$ generated by eq. (1.1) form a subspace H_Φ of the complete Hilbert space H. Solving eq. (1.3) is equivalent to diagonalizing the Hamiltonian H in the subspace H_Φ. The GCM would give an exact solution if all N-particle states could be generated by the integral (1.1), i.e. if $H_\Phi = H$. In other

cases the method gives approximate eigenfunctions and eigenvalues and the accuracy of the method depends on the extent to which the studied eigenstates of H can be approximated by states in H_Φ. This in turn depends on the choice of the generating functions $\Phi(x,\alpha)$.

From the physical point of view, the GCM offers efficient method how to build in some informations obtained from experiments or from models about the system. From the mathematical point of view, however, the continuous and nonorthogonal basis of the GCM is sometimes less convenient to work with than orthogonal bases one normally uses in the diagonalization of the Hamiltonian. It seems to us, that the existing evidence (see Chapters 3 and 4) supports the feeling that the GCM represents an efficient method which overcompensates mathematical complications if the informations used are relevant.

The Proceedings is divided in three chapters. In the Chapter 2 "General Theory and Mathematical Problems" the emphasis is:
(i) on those attempts which try to come as far as possible analytically. In order to do this one approximates the kernels $I(\alpha,\alpha')$ and $H(\alpha,\alpha')$, eq. (1.4), by a Gaussian function of $(\alpha-\alpha')$ times a polynomial. Then one can do algebraic manipulations (equivalent to) boson expansions and the numerical calculation comes only at a late stage. The above method means that the original many body problem is replaced by a different problem.
(ii) Those attempts which can be performed entirely numerically. In this case one does not "deform" the original many body problem, however, one solves the problem approximately in a truncated space spanned by vectors having a not too small norm. The method is probably suitable for systems having small number of degrees of freedom which have to be treated more accurately.

In the Chapter 3 "Bound States" the emphasis is on those examples of the application of the GCM to the situations in which other methods failed to provide a completely satisfactory description. Some of these applications were already published, some

others seem tractable by the (slightly modified) existing programs for the projection of angular momentum and the number of particles. The present activity in the GCM is partly due to the existence of the advanced projection "technology".

The application of the GCM to nuclear reactions is still at a pioneering stage, so far only some schematic examples were treated. In Chapter 4 the emphasis is: (i) on handling the scattering boundary conditions and solving the corresponding Schrödinger equation and (ii) on the formulation of models for semirealistic calculations.

2. GENERAL THEORY AND MATHEMATICAL PROBLEMS

2.1. Some properties of solutions of the Hill-Wheeler equation

Symmetry of solutions. The exact eigenstates of H are also eigenstates of some others operators whereas the generating functions $\Phi(x,\alpha)$ usually have less symmetry than the exact eigenstates. Approximate eigenstates of H generated by the GCM will be eigenstates of symmetry operators only if the set of functions $\Phi(x,\alpha)$ are complete in the sense that [2)]

$$S\Phi(x,\alpha) = \Phi(x,\sigma(\alpha)) \ , \tag{2.1}$$

Where S and σ are the respective symmetry operators.

Some consequences of the nonorthogonal and continuous basis. There are two problems in connection with the amplitude function $f(\alpha)$:

1. It can happen that for well-behaved N-particle functions $\Psi(x)$ and generating functions $\Phi(x,\alpha)$ the corresponding $f(\alpha)$ are highly singular distributions (see also section (2.2.1)).
2. Due to the nonorthogonality of the basis $\Phi(x,\alpha)$ we cannot interpret $|f(\alpha)|^2$ as the probability w_α of finding the component $\Phi(x,\alpha)$ in the state $\Psi(x)$. Instead, the probability w_α is connected with

$$I\ f = \int I(\alpha,\alpha')f(\alpha')d\alpha' = \langle\Phi(x,\alpha)|\Psi\rangle \ . \tag{2.2}$$

The above mentioned difficulties suggest to introduce

$$F(\alpha) = I\ f \tag{2.3}$$

The function $F(\alpha)$ will be a well-behaved function even if $f(\alpha)$ is singular, and it has a direct physical interpretation;

it has been used both in bound state [3,4] and scattering problems [5]. A drawback of using $F(\alpha)$ is that, due to the non-orthogonality of $\Phi(x,\alpha)$, the "probabilities" $w_\alpha = |F(\alpha)|^2$ do not add up to 1.

An alternative representation. Some of the above difficulties can be remedied by switching to [2]

$$g = I^{1/2} f \ . \tag{2.4}$$

The functions g generated in this way form a subspace H_g. From (1.1) and (2.4) together with (1.4) it is easy to prove that the connection between H_g and the subspace H_Φ, generated by the GCM, is unitary. We write

$$\Psi = U\, g \tag{2.5}$$

U being a unitary operator. The transformation U also establishes a correspondence between operators acting in H_Φ and operators in H_g. For example, if H is the complete Hamiltonian of the N-particle system, Ψ_μ and Ψ_ν arbitrary states in H_Φ, g_μ and g_ν the corresponding states in H_g, we can define an "equivalent" Hamiltonian $\hat{h}$ in H_g by its matrix elements

$$\langle g_\mu | \hat{h} | g_\nu \rangle = \langle \Psi_\mu | H | \Psi_\nu \rangle \ . \tag{2.6}$$

Solving (1.3) is then equivalent to diagonalizing $\hat{h}$ in H_g, i.e. to solving the eigenvalue problem

$$\hat{h} g = E g \tag{2.7}$$

Eq. (2.7) is only useful if we can construct $\hat{h}$ explicitly and if $\hat{h}$ has a simple structure. The general procedure for converting (1.3) into (2.7) could be the following:

i) Find a function $I^{1/2}(q,\alpha) \equiv \chi(q,\alpha)$ so that *

$$I(\alpha,\alpha') = \int \chi^*(q,\alpha)\chi(q,\alpha')dq \qquad (2.8)$$

Eq. (1.3) can then be rewritten as

$$\iint \chi^*(q,\alpha')\{h(\alpha',\alpha) - E\}\, \chi(q,\alpha)f(\alpha)d\alpha\, dq = 0 \qquad (2.9)$$

where

$$h(\alpha',\alpha) \equiv H(\alpha',\alpha)/I(\alpha',\alpha)\ . \qquad (2.10)$$

ii) Find operators $\hat{b}(q,\partial/\partial q)$ so that

$$\hat{b}\chi(q,\alpha) = \alpha\, \chi(q,\alpha)\ . \qquad (2.11)$$

iii) Replace in the Taylor expansion of $h(\alpha',\alpha)$ each α by $\hat{b}$ and each α' by $\hat{b}^+$ where the order is such that $\hat{b}^+$ is always on the left (normal order, denoted by :( ):). One can then introduce

$$g(q) = \int \chi(q,\alpha)\, f(\alpha)\, d\alpha \qquad (2.4')$$

and eq.(2.9) transforms into (2.7) with

$$\hat{h} = :\, h(\hat{b}^+,\hat{b}):\ . \qquad (2.12)$$

An example for this procedure will be given in the following sections.

* There is one q-variable for each generator coordinate α. Indices labelling different generator coordinates α_i are omitted.

2.2. Present status

2.2.1. A soluble model: Gaussian overlap approximations (GOA).

We make the assumption (to be discussed in Section 2.2.2.) that

$$I(\alpha',\alpha) = \exp\{-\frac{1}{2}\, s(\alpha' - \alpha)^2\} \qquad (2.13)$$

$$h(\alpha',\alpha) = E(0) + \frac{1}{2}\,(\alpha B\alpha + \alpha' B^*\alpha' + 2\alpha' A\alpha)\ , \qquad (2.14)$$

where * means complex conjugate. From the Hermiticity of H it follows that the matrix B is symmetric and A Hermitian. If (2.13) holds one finds immediately as a solution of eq. (1.12)

$$\chi(q,\alpha) = C\, \exp\{-s(q - \alpha)^2\};\ -\infty < q < +\infty \qquad (2.15)$$

The operators $\hat{b}^+$ and $\hat{b}$ of eq. (2.11) can be expressed as

$$\hat{b} = q + \frac{1}{2s}\frac{\partial}{\partial q}\ ;\ \hat{b}^+ = q - \frac{1}{2s}\ \frac{\partial}{\partial q}\ . \qquad (2.16)$$

They obey Boson commutation rules. Inserting (2.14) and (2.15) into (2.9) and making use of the relation

$$\int d\,q\ \ldots\ \hat{b}\ \chi(q,\alpha) = \int d\,q\ \ldots\ \alpha\ \chi(q,\alpha) \qquad (2.17)$$

and the adjoint relation

$$\int d\,q\ \chi^*(q,\alpha')\ \hat{b}^+\ \ldots = \int d\,q\ \chi^*(q,\alpha')\alpha'\ \blacksquare \qquad (2.18)$$

one gets the Hamiltonian $\hat{h}$, eq. (2.6), as a quadratic form of the "creation" and "annihilation" operators $\hat{b}$, $\hat{b}^+$:

$$\hat{h} = E(0) + \frac{1}{2}(\hat{b}^+ B\hat{b}^+ + \hat{b}B^*\hat{b} + 2\hat{b}^+ A\hat{b})\ . \qquad (2.19)$$

The explicit formulae for $s, E(0)$, A and B are

$$s = \langle \partial\Phi | \partial\Psi \rangle_{\alpha=0} \tag{2.20}$$

$$E(0) = \langle \Psi | H | \Phi \rangle_{\alpha=0}; \quad A = \langle \partial\Phi | H - E(0) | \partial\Phi \rangle_{\alpha=0}; \quad B = \langle \partial^2\Phi | H - E(0) | \Phi \rangle_{\alpha=0} \tag{2.21}$$

where the notation $\partial^n\Psi = \partial^n\phi/\partial\alpha^n$ is used.

To solve (2.7) with $\hat{h}$ from eq. (2.19) we introduce new operators

$$\hat{Q}^+ = x\hat{b}^+ - y\hat{b} \tag{2.22}$$

where x and y are determined by

$$[\hat{h}, \hat{Q}^+] = \varepsilon \hat{Q}^+ . \tag{2.23}$$

The adjoint of this relation is $[\hat{h}, \hat{Q}] = -\varepsilon\hat{Q}$.
The eigenvalue ε can be interpreted as the excitation energy. The ground state g_o is determined by the relation $\hat{Q}g_o = 0$ and excited states by $g_n = (\hat{Q}^+)^n g_o$.

The resulting equations for x,y

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} = \varepsilon \begin{pmatrix} x \\ -y \end{pmatrix} \tag{2.24}$$

have the same structure as the equations of the random phase approximation (RPA). They are identical with RPA if we choose α to be the particle-hole amplitudes c_{mi} in

$$|\Phi(x,\alpha)\rangle = \exp\{ \sum_{\substack{m>N \\ i\leq N}} \alpha_{mi}\, c_m^+\, c_i \}|0\rangle \tag{2.25}$$

The matrix in the eq. (2.24) is not Hermitian and the

eigenvalues may be complex. There is, however, a theorem by Thouless [6] saying that a necessary and sufficient condition for ε to be real is that the matrix $\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}$ is nonnegative. We can fulfill this condition by introducing complex parameters (the parameter α' is replaced by α'^*). The integration in (1.1) is then taken over $\mathrm{Re}\alpha$ and $\mathrm{Im}\alpha$ separately. We require that the expectation value $H(\alpha,\alpha)$ has a minimum at $\alpha = 0$, i.e. $H(\alpha,\alpha) \geq H(0,0)$ for arbitrary small complex value of α. This condition is sufficient [6] to ensure in the expansion (2.14) no terms linear in α and α' appear and that $\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}$ is non-negative. If we restrict ourselves to real parameters α then the stability of the state $\Phi(x,0)$ means that the matrix $(B + B^* + 2A)$ has to be nonnegative. No conclusion about the reality of the eigenvalues ε of eq. (2.24) can be drawn from the latter condition.

There is one more reason in favour of extending the GCM to complex parameters α. With real parameters it turns out that the space H^g generated by eq. (2.4) in general does not contain all square integrable function $g(q)$. Hence it can happen that there is no amplitude function $f(\alpha)$ which generates the eigenstates of the equivalent Hamiltonian $\hat{h}$. For example [2] the one-parametric function

$$g(q) = \exp(-\gamma q^2) \tag{2.26}$$

is square integrable in H_g if $\mathrm{Re}\gamma > 0$ but can be represented as an integral

$$g(q) = \int \exp(-s\,(q - \alpha)^2) f(\alpha)\, d\alpha;\ \alpha \text{ and } s \text{ are real} \tag{2.27}$$

with regular $f(\alpha)$ only if also $\mathrm{Re}\gamma < s$. For $\mathrm{Re}\gamma = s$, $f(\alpha)$ becomes a δ-function and for $\mathrm{Re}\gamma > s$ one would have to introduce a highly singular distribution "worse" than the δ-function. If, on the other hand, one makes the extension to complex parameters α as described above, then the amplitude function $f(\alpha)$ in (2.27) can

always be represented as an analytic function in α. It is an open problem whether complex parameters also help if $\chi(q,\alpha)$ has a more general form than (2.15).

2.2.2. Approaches to anharmonic oscillations

2.2.2.1. Small anharmonic corrections

In order to go beyond the Gaussian overlap and harmonic approximation one has to expand the kernels $I(\alpha',\alpha)$ and $H(\alpha',\alpha)$ to higher terms than in (2.13) and (2.14). We shall write the expansion for a single generator coordinate, the generalization to more than one generator coordinate is straightforward.

We shall assume, that the functions $\Phi(\alpha)$ are real and normalized to unity.

$$\langle\Phi(\alpha')|\Phi(\alpha)\rangle = \exp\left[-\frac{1}{2}\, s\,(\alpha-\alpha)^2\right]$$

$$\cdot\left[1 + \tilde{N}^{(3)}(\alpha'^3 - \alpha'^2\alpha - \alpha'\alpha^2 + \alpha^3) + \tilde{N}_o^{(4)}(\alpha'^4 + \alpha^4)\right. \tag{2.28}$$

$$\left. + \tilde{N}_1^{(4)}(\alpha'^3\alpha + \alpha'\alpha^3) + 2\tilde{N}_2^{(4)}\,\alpha'^2\alpha^2 + \ldots\right]$$

Here, the parameter s is still given by eq. (2.20) and the expansion coefficients $\tilde{N}_i^{(\nu)}$ are

$$\tilde{N}^{(3)} = -\frac{1}{2}\langle\partial^2\Phi|\partial\Phi\rangle_{(\alpha=o)}\,, \tag{2.29}$$

$$\tilde{N}_o^{(4)} = \left[-\frac{1}{6}\langle\partial^3\Phi|\partial\Phi\rangle - \frac{1}{8}\langle\partial^2\Phi|\partial^2\Phi\rangle - \frac{1}{8}\langle\partial\Phi|\partial\Phi\rangle^2\right]_{(\alpha=o)} \tag{2.30}$$

$$\tilde{N}_1^{(4)} = \left[\frac{1}{6}\langle\partial^3\Phi|\partial\Phi\rangle + \frac{1}{2}\langle\partial\Phi|\partial\Phi\rangle^2\right]_{(\alpha=o)}\,, \tag{2.31}$$

$$\tilde{N}_2^{(4)} = \left[\frac{1}{8}\langle\partial^2\Phi|\partial^2\Phi\rangle - \frac{3}{8}\langle\partial\Phi|\partial\Phi\rangle^2\right]_{(\alpha=o)}\,, \tag{2.32}$$

The relations

$$\langle \partial^2\Phi | \Phi\rangle + \langle \partial\Phi | \partial\Phi\rangle = 0 \ ,$$

$$\langle \partial^3\Phi | \Phi\rangle + 3\langle \partial^2\Phi | \partial\Phi\rangle = 0 \ ,$$

$$\langle \partial^4\Phi | \Phi\rangle + 4\langle \partial^3\Phi | \partial\Phi\rangle + 3\langle \partial^2\Phi | \partial^2\Phi\rangle = 0 \ ,$$

which follow from the normalization condition for Φ, were taken into account.

Similarly,

$$h(\alpha',\alpha) = \langle\Phi(\alpha')|H|\Phi(\alpha)\rangle / \langle\Phi(\alpha')/\Phi(\alpha)\rangle =$$

$$= E(0) + A\alpha\alpha' + \frac{1}{2} B(\alpha^2 + \alpha'^2) + C_o^{(3)}(\alpha'^3 + \alpha^3) +$$

$$+ C_1^{(3)}(\alpha'^2\alpha + \alpha'\alpha^2) + C_o^{(4)}(\alpha'^4 + \alpha^4) +$$

$$+ C_1^{(4)}(\alpha'^3\alpha + \alpha'\alpha^3) + 2C_2^{(4)}\,\alpha'^2\alpha^2 + \ldots \ , \qquad (2.33)$$

where $E(0)$, A and B are still given by eqs. (2.21) and

$$C_o^{(3)} = \frac{1}{3!}\langle \partial^3\Phi | H - E(0) | \Phi\rangle_{(\alpha=o)} \qquad (2.34)$$

$$C_1^{(3)} = \frac{1}{2!}\langle \partial^2\Phi | H - E(0) | \partial\Phi\rangle_{(\alpha=o)} \qquad (2.35)$$

$$C_o^{(4)} = \left[\frac{1}{4!}\langle \partial^4\Phi | H - E(0) | \Phi\rangle + \frac{1}{4} E(0)\langle \partial\Phi | \partial\Phi\rangle^2\right]_{(\alpha=o)} \qquad (2.36)$$

$$C_1^{(4)} = \left[\frac{1}{3!}\langle \partial^3\Phi | H - E(0) | \partial\Phi\rangle - E(0)\,\langle \partial\Phi | \partial\Phi\rangle^2\right]_{(\alpha=o)} \qquad (2.37)$$

$$C_2^{(4)} = \left[\frac{1}{4}\langle \partial^2\Phi | H - E(0) | \partial^2\Phi\rangle + \frac{3}{2} E(0)\,\langle \partial\Phi | \partial\Phi\rangle^2\right]_{(\alpha=o)} \qquad (2.38)$$

In order to verify whether the Gaussian overlap and harmonic approximation is a good zeroth order approximation upon which small anharmonic corrections are to be added, one has to look in practi-

cal cases at the expansion coefficients $\tilde{N}_i^{(\nu)}$ and $C_i^{(\nu)}$. The series (2.28) and (2.33) should converge for values of α,α' of the order $1/\sqrt{s}$ as will be seen later, (2.53). There is, however, a general argument supporting the validity of GOA. This argument is valid only in the limit of a large number of particles, but it may have some qualitative relevance for nuclear physics. We discuss briefly the situation in which $\Phi(\alpha)$ is a Slater determinant of single particle wave functions $\phi_i(\alpha) \equiv \phi_i(x;\alpha)$. Here x stands for the set of all coordinates of a single particle. Then the overlap integral $I(\alpha',\alpha)$ may be expressed in terms of the matrix

$$n_{i,j}(\alpha',\alpha) = \langle\phi_i(\alpha')|\phi_j(\alpha)\rangle \ . \qquad (2.39)$$

Indeed we may write

$$I(\alpha',\alpha) \equiv \det n(\alpha',\alpha) = \exp\{\mathrm{tr}\ \log n(\alpha',\alpha)\}. \qquad (2.40)$$

When the number N of particles participating in a given mode is large, the quantity tr log $n(\alpha',\alpha)$ very quickly becomes large (of the order N) and negative, as soon as α' deviates from α by an amount of the order of $1/\sqrt{s_o}$ (typical width of the single-particle overlaps $n_{ij}(\alpha',\alpha)$). This follows from the fact that the matrix $n(\alpha',\alpha)$ cannot have eigenvalues larger than unity and from the assumption that for $|\alpha-\alpha'| \sim 1/\sqrt{s_o}$ a very large number of the eigenvalues will actually be smaller than unity by an amount of the order of unity.

If one expands*

$$\log\langle\Phi(\alpha')|\Psi(\alpha)\rangle \equiv \mathrm{tr}\ \log n(\alpha',\alpha) = -\frac{1}{2}\, s(\alpha-\alpha')^2 +$$

$$+ N^{(3)}(\alpha'^3 - \alpha'^2\alpha - \alpha'\alpha^2 + \alpha^3) + N_o^{(4)}(\alpha'^4 + \alpha^4) +$$

$$+ N_1^{(4)}(\alpha'^3\alpha + \alpha'\alpha^3) + 2N_2^{(4)}\,\alpha'^2\alpha^2 + \ldots \qquad (2.41)$$

*The expansion coefficients $N_i^{(\nu)}$ coincide with $\tilde{N}_i^{(\nu)}$, eq. (2.26), up to 4th order.

it follows that each expansion coefficient $N_i^{(\nu)}$ is separately of the order $N.s_o^{\nu/2}$. In particular, $s \equiv N^{(2)} \sim N\, s_o$.

As will be seen later (2.53), the relevant range of α (the width of the Hill-Wheeler amplitude function) is of the order of $1/\sqrt{s}$ if the GOA is a good starting point. Then $\frac{1}{\sqrt{s}} \sim \frac{1}{\sqrt{N}} \cdot \frac{1}{\sqrt{s_o}}$ so that the series (2.41) is in fact expanded in powers of $1/\sqrt{N}$. It is convenient to keep the quadratic term in (2.41) in the exponential and to expand further terms in the form (2.28). Similarly, the Hamiltonian overlap (2.33) is also expanded in powers of $1/\sqrt{N}$.

Coming back to the approach, proposed in Section 2.1, we write

$$\int \left[h'(\alpha',\alpha) - E i'(\alpha',\alpha)\right] \exp\left\{-\frac{1}{2}\, s(\alpha' - \alpha)^2\right\} f(\alpha)\, d\alpha = 0 \quad , \qquad (2.42)$$

where i' is polynomial in α and α', appearing in eq. (2.28), and h' is the product of i' times the right hand side of eq. (2.33).

In order to transform eq. (2.42) into a differential equation we replace the Gaussian factor $\exp\left[-\frac{1}{2}\, s(\alpha - \alpha')^2\right]$ by its decomposition provided by eqs. (2.8) and (2.15). Following the method described in Section 2.1., we write the factor $\chi^*(q,\alpha')$ to the left and the factor $\chi(q,\alpha)$ to the right of the bracket [ ] in eq. (2.42). Finally we replace the quantities α' and α by the operators $\hat{b}$ and $\hat{b}^+$, respectively, rewritten in normal order. In this way we arrive at the differential equation

$$\left[\hat{h}' - E\hat{i}'\right] g'(q) = 0 \qquad (2.43)$$

where $g'(q)$ is given by eq. (2.4') with $\chi(q,\alpha)$ as in eq. (2.15). The operators $\hat{h}'$ and $\hat{i}'$ can be expanded either up to a given order in operators $\hat{b}$ *or* up to a given order in $1/\sqrt{N}$, depending on the actual value of the expansion coefficients. Here, we present the latter expansion up to $(1/\sqrt{N})^2$.

$$\hat{i}' = :i'(\hat{b}^+,\hat{b}): = 1 + N^{(3)}(\hat{b}^{+3}+\hat{b}^3-\hat{b}^{+2}\hat{b}-\hat{b}^+\hat{b}^2)$$
$$+ N_o^{(4)}(\hat{b}^{+4}+\hat{b}^4) + N_1^{(4)}(\hat{b}^{+3}\hat{b}+\hat{b}^+\hat{b}^3) + 2N_2^{(4)}\hat{b}^{+2}\hat{b}^2$$
$$+ \frac{1}{2}(N^{(3)})^2(\hat{b}^{+6}+\hat{b}^6-2\hat{b}^{+5}\hat{b}-2\hat{b}^+\hat{b}^5-\hat{b}^{+4}\hat{b}^2-\hat{b}^{+2}\hat{b}^4+4\hat{b}^{+3}\hat{b}^3) \qquad (2.44)$$

$$\hat{h}' = :h'(\hat{b}^+,\hat{b}): = E(0)\hat{i}'+A\hat{b}^+\hat{b}+\frac{1}{2}B(\hat{b}^{+2}+\hat{b}^2)$$
$$+ C_o^{(3)}(\hat{b}^{+3}+\hat{b}^3) + C_1^{(3)}(\hat{b}^{+2}\hat{b}+\hat{b}^+\hat{b}^2)$$
$$+ C_o^{(4)}(\hat{b}^{+4}+\hat{b}^4) + C_1^{(4)}(\hat{b}^{+3}\hat{b}+\hat{b}^+\hat{b}^3) + 2C_2^{(4)}\hat{b}^{+2}\hat{b}^2$$
$$+ \frac{1}{2}N^{(3)}B(\hat{b}^{+5}+\hat{b}^5) + N^{(3)}(A-\frac{1}{2}B)(\hat{b}^{+4}\hat{b}+\hat{b}^+\hat{b}^4)$$
$$- N^{(3)}A(\hat{b}^{+3}\hat{b}^2+\hat{b}^{+2}\hat{b}^3) + (\frac{1}{2}N_o^{(4)}B+N^{(3)}C_o^{(3)})(\hat{b}^{+6}+\hat{b}^6)$$
$$+ (N_o^{(4)}A+\frac{1}{2}N_1^{(4)}B+N^{(3)}C_1^{(3)}-N^{(3)}C_o^{(3)})(\hat{b}^{+5}\hat{b}+\hat{b}^+\hat{b}^5)$$
$$+ (\frac{1}{2}N_o^{(4)}B+N_1^{(4)}A+N_2^{(4)}B-N^{(3)}C_o^{(3)})(\hat{b}^{+4}\hat{b}^2+\hat{b}^{+2}\hat{b}^4)$$
$$+ 2(\frac{1}{2}N_1^{(4)}B+N_2^{(4)}A+N^{(3)}C_o^{(3)}-N^{(3)}C_1^{(3)})\hat{b}^{+3}\hat{b}^3$$
$$+ \frac{1}{4}(N^{(3)})^2B(\hat{b}^{+8}+\hat{b}^8)+\frac{1}{2}(N^{(3)})^2(A-B)(\hat{b}^{+7}\hat{b}+\hat{b}^+\hat{b}^7)$$
$$- (N^{(3)})^2A(\hat{b}^{+6}\hat{b}^2+\hat{b}^{+2}\hat{b}^6)+\frac{1}{2}(N^{(3)})^2(B-A)(\hat{b}^{+5}\hat{b}^3+\hat{b}^{+3}\hat{b}^5)$$
$$+ (N^{(3)})^2(2A-\frac{1}{2}B)\hat{b}^{+4}\hat{b}^4 \ . \qquad (2.45)$$

Instead of solving eq. (2.43), we might prefer to solve the equation

$$(\hat{h} - E)g(q) = 0 \qquad (2.46)$$

where

$$\hat{h} = \hat{i}'^{-1/2}\,\hat{h}'\hat{i}'^{-1/2} \qquad (2.47)$$

$$g(q) = \hat{i}'^{1/2}\,g'(q) \qquad (2.48)$$

The operator $\hat{h}$ has for example a much simpler expression than the operator $\hat{h}'$ in the simple model of Lipkin [9,10].

The boson expansions (2.44), (2.45) obtain a simpler form if the generating function is of any one of the following two types:

$$\Phi(\alpha) = \frac{e^{\alpha A^+}\phi(0)}{\langle\phi(0)|e^{\alpha A}e^{\alpha A^+}|\phi(0)\rangle}, A\phi(0) = 0 , \qquad (2.49)$$

or

$$\Phi(\alpha) = e^{i\alpha A}\,\phi(0) , \quad A^+ = A . \qquad (2.50)$$

Often we assume A to be a one body operator and $\phi(0)$ to be a Slater determinant. When eq. (2.49) applies we have

$$N^{(3)} = N_1^{(4)} = 0$$

$$N_0^{(4)} = N_2^{(4)} = \frac{1}{8}\left[\langle\phi(0)|A^2A^{+2}|\phi(0)\rangle - 2\langle\phi(0)|AA^+|\phi(0)\rangle^2\right] .$$

When eq. (2.50) applies we have

$$N_0^{(4)} = -\frac{1}{4}N_1^{(4)} = \frac{1}{3}N_2^{(4)} = \frac{1}{24}\left[\langle\phi(0)|A^4|\phi(0)\rangle - 3\langle\phi(0)|A^2|\phi(0)\rangle^2\right].$$

It is not possible to solve eq.(2.43) analytically, but the numerical work left over is hopefully much smaller than in an entirely numerical procedure. A rough approximation was suggested in ref. [10]

2.2.2.2. Strongly anharmonic oscillations

Strongly anharmonic collective oscillations arise when the RPA energy is zero,

$$\varepsilon = \sqrt{A^2 - B^2} = 0 ; \qquad (2.51)$$

where A and B are given by eq. (2.21). In the harmonic approximation, assuming also $B^* = B$, the Hamiltonian may be written

$$\hat{h} = E(0) - \frac{1}{4}(A-B)(\hat{b}^+ - \hat{b})^2 + \frac{1}{4}(A+B)(\hat{b}^+ + \hat{b})^2 - \frac{1}{2}A$$

$$= E(0) - \frac{1}{2}A - \frac{1}{4s^2}(A-B)\frac{\partial^2}{\partial q^2} + (A+B)q^2 \ . \qquad (2.52)$$

If $B = -A$ the quadratic approximation to the "potential energy" $(A+B)q^2$ is not valid. If $B = A$, it is the quadratic approximation to the "kinetic energy" $-(1/4s^2)(A-B)\,\partial^2/\partial q^2$ which is not valid. A deeper insight into this problem is provided by the consideration of the expectation values $\langle q^2 \rangle$, $\langle -\partial^2/\partial q^2 \rangle$ for the ground state of $\hat{h}$. We have

$$\langle q^2 \rangle = \frac{1}{4s}\sqrt{\frac{A-B}{A+B}} \ , \quad \langle -\frac{\partial^2}{\partial q^2} \rangle = s\sqrt{\frac{A+B}{A-B}} \ . \qquad (2.53)$$

When the RPA breaks down we have therefore either $\langle q^2 \rangle = \infty$, $\langle -\partial^2/\partial q^2 \rangle = 0$ or $\langle -\partial^2/\partial q^2 \rangle = \infty$, $\langle q^2 \rangle = 0$. It is, of course, the first case that we would like to have, because then we may still hope that the quadratic approximation for the kinetic energy is appropriate. It may be observed here that the amplitude function $f(\alpha)$ corresponding to eigenstates of $\hat{h}$ is a well behaved function if* $4s^2 \langle q^2 \rangle > \langle -\partial^2/\partial q^2 \rangle$, what is equivalent to $\frac{(A-B)}{(A+B)} > \frac{(A+B)}{(A-B)}$. We will now show that it is always possible to fulfil the above condition. For this purpose we replace the generating function $\Phi(\alpha)$ by $\Phi(e^{i\phi}\alpha)$, with ϕ real. We are thus replacing the real generator coordinate α by a complex quantity, but in contrast to the program proposed at the end of Section 2.1.1, now we are only considering linear combinations of $\Phi(\alpha)$ along a well defined direction in the α complex plane. The operator

*After some manipulation this condition can be traced back to $\mathrm{Re}\gamma < s$ at the end of Section 2.1.1.

$\hat{h}$ of eq. (2.52) is replaced by

$$\hat{h} = E(0) + A\hat{b}^{+}\hat{b} + \frac{1}{2} B(e^{-2i\phi}\hat{b}^{+2} + e^{2i\phi}\hat{b}^{2}) \tag{2.54}$$

so that eq. (2.53) becomes

$$\begin{aligned} \langle q^2 \rangle &= \frac{1}{4s} \sqrt{\frac{A-B\cos 2\phi}{A+B\cos 2\phi}} \\ \left\langle -\frac{\partial^2}{\partial q^2} \right\rangle &= s \sqrt{\frac{A+B\cos 2\phi}{A-B\cos 2\phi}} \end{aligned} \tag{2.55}$$

By chosing an appropriate ϕ we can always insure that $4s^2\langle q^2 \rangle > \langle -(\partial^2/\partial q^2) \rangle$. Actually ϕ should be chosen so that $\langle -(\partial^2/\partial q^2 \rangle$ is as small as possible. If the harmonic approximation breaks down, the fluctuation in q is then very large and the "potential energy" must be written as a general function of q. Hopefully we can still use the quadratic approximation for the "kinetic energy".

These ideas can be realized by the following approximations

$$\langle \Phi(\alpha') | \Phi(\alpha) \rangle = \exp\left[-\frac{1}{2} S\left(\frac{\alpha+\alpha'}{2}\right) [\alpha - \alpha']^2 \right] \tag{2.56}$$

$$h(\alpha',\alpha) = \mathcal{E}\left(\frac{\alpha+\alpha'}{2}\right) - \frac{1}{2}(\alpha-\alpha')^2 M\left(\frac{\alpha+\alpha'}{2}\right) \tag{2.57}$$

where

$$S(\alpha) = \langle \partial\Phi(\alpha) | \partial\Phi(\alpha) \rangle \tag{2.58}$$

$$\mathcal{E}(\alpha) = h(\alpha,\alpha) \tag{2.59}$$

$$M(\alpha) = \left[\frac{\partial^2 h(\alpha',\alpha)}{\partial\alpha\, \partial\alpha'} - \frac{\partial^2 h(\alpha',\alpha)}{\partial\alpha^2} \right]_{(\alpha=\alpha')} . \tag{2.60}$$

Since $h(\alpha,\alpha') = h(\alpha',\alpha)$, no linear terms in $(\alpha-\alpha')$ appear. Again,

we have assumed that $\Phi(\alpha)$ is real and normalized to unity. As explained elsewhere [11], we can always make a transformation of the generator coordinate $\beta = \beta(\alpha)$ so that $S(\beta)$ is constant. In the following it will be assumed that the coordinate α has been chosen so that $S(\alpha) \equiv 1$.

The Hill-Wheeler equation becomes now

$$\int \left[\mathcal{E}\left(\frac{\alpha+\alpha'}{2}\right) - \frac{1}{2}(\alpha-\alpha')^2 M\left(\frac{\alpha+\alpha'}{2}\right) - E\right] e^{-\frac{1}{2}(\alpha-\alpha')^2} f(\alpha)\,d\alpha = 0 \qquad (2.61)$$

Following the arguments of ref. [11] this equation may be replaced by the differential equation

$$\left\{ -\frac{1}{4}\left[\hat{b}^{+2}\tilde{M}\left(\frac{\hat{b}^+ + \hat{b}}{2}\right) - 2\hat{b}^+\tilde{M}\left(\frac{\hat{b}^+ + \hat{b}}{2}\right)\hat{b} + \tilde{M}\left(\frac{\hat{b}^+ + \hat{b}}{2}\right)\hat{b}^2\right] + \tilde{\mathcal{E}}\left(\frac{\hat{b}^+ + \hat{b}}{2}\right) - E\right\} g(q) = 0\,, \qquad (2.62)$$

where the function $\tilde{M}$ is related to the function M by

$$\tilde{M}(u) = M(u) - \frac{1}{8}\frac{\partial^2 M}{\partial u^2} + \ldots + (-1)^k \frac{1}{k!\,8^k}\frac{\partial^{2k} M}{\partial u^{2k}} + \cdots \qquad (2.63)$$

where u is a dummy variable. A similar expression holds for $\tilde{\mathcal{E}}(u)$.

Finally we may give to eq. (2.62) the form of a general oscillator

$$\left\{-\frac{1}{4}\frac{\partial}{\partial q}\tilde{M}(q)\frac{\partial}{\partial q} - \frac{1}{16}\frac{\partial^2 \tilde{M}(q)}{\partial q^2} - \frac{1}{4}\tilde{M}(q) + \tilde{\mathcal{E}}(q) - E\right\} g(q) = 0 \qquad (2.64)$$

Although there is no clear cut separation between potential and kinetic energy terms, it seems instructive to interpret $\tilde{M}$ as the mass parameter and $\tilde{\mathcal{E}}$ as the potential energy. In the special case of the harmonic approximation, which means neglecting derivatives of $h(\alpha,\alpha')$ of higher order than the second, $\tilde{M}(q) \to M(0) = A-B$,

$$\frac{\partial^2 M(q)}{\partial q^2} \longrightarrow 0$$

$$\tilde{\mathcal{E}}(q) \longrightarrow \tilde{\mathcal{E}}(0) + \frac{1}{2} q^2 \frac{\partial^2 \tilde{E}}{\partial q^2} = \mathcal{E}(0) - \frac{1}{8} \frac{\partial^2 \mathcal{E}}{\partial q^2} + \frac{1}{2} q^2 \frac{\partial^2 \mathcal{E}}{\partial q^2}$$

$$= \mathcal{E}(0) - \frac{1}{4} (A+B) + q^2 (A+B) .$$

Eq. (2.64) then reduces to eq. (2.52).

2.2.2.3. Other approaches to the boson expansion problem

Several authors have considered the problem of boson expansions of operators refering to fermion systems [12,13,14]. Recently, Jansen et al. [16] and Holzwarth [4] were able to establish a connection between the boson expansion of Marumori [13] and the boson expansion for a generating function of the Jancovici-Schiff type [3].

We will briefly describe the work of Holzwarth, since it is somewhat connected with the approach described in section 2.2.2.1. Holzwarth considers a generating function of the Jancovici-Schiff type

$$|\alpha\rangle = \exp\left[\sum_{m,i} \alpha_{mi} c_m^+ c_i^+\right]|0\rangle \ , \ c_m|0\rangle = 0, \ c_i^+|0\rangle = 0 \ .$$

The Hill-Wheeler equation

$$\int \left[\langle\alpha'|H|\alpha\rangle - E\langle\alpha'|\alpha\rangle\right] f(\alpha)d\alpha = 0$$

involves the overlap integrals

$$H(\alpha',\alpha) = \langle\alpha'|H|\alpha\rangle \ , \ I(\alpha',\alpha) = \langle\alpha'|\alpha\rangle \ .$$

The following quantities

$$h'(\alpha',\alpha) = H(\alpha',\alpha)e^{-\alpha'^*\alpha}$$

$$i'(\alpha',\alpha) = I(\alpha',\alpha)e^{-\alpha'^*\alpha} \ .$$

$$\alpha'^*\alpha = \sum_{m,i} \alpha'^*_{mi}\,\alpha_{mi}$$

are then introduced, so that the Hill-Wheeler equation becomes

$$\int \left[h'(\alpha',\alpha) - Ei'(\alpha',\alpha)\right] e^{\alpha'^*\alpha}\, f(\alpha)d\alpha = 0 \ .$$

This integral equation is transformed into a differential equation by introducing operators B^+_{mi}, B_{mi} which act on functions of α'_{mi} ,

$$B_{mi} = \frac{\partial}{\partial\alpha'_{mi}} \ , \quad B^+_{mi} = \alpha'_{mi} \ .$$

We obtain in this way

$$\left[\hat{h}'(B^+,B) - E\hat{i}'(B^+,B)\right] \int e^{\alpha'^*\alpha}\, f(\alpha)d\alpha = 0$$

where

$$\hat{h}'(B^+,B) = :h'(B^+,B):$$

$$\hat{i}'(B^+,B) = :i'(B^+,B): \ .$$

Both $\hat{h}'$ and $\hat{i}'$ are zero in the spurious subspace of Marumori (the orthogonal complement to the physical subspace) and have zero matrix elements between the physical and the spurious subspace. Moreover it may be seen that the basis which has been used to define the physical subspace diagonalises the operator $\hat{i}'$. The operator $(\hat{i}')^{-1/2}$ is therefore easily computed and finally it can be shown that the operator

$$\hat{h}(B^+,B) = \left[\hat{i}'(B^+,B)\right]^{-1/2} \hat{h}'(B^+,B)\left[\hat{i}'(B^+,B)\right]^{-1/2} \ .$$

which is well defined in the physical subspace, coincides with Marumori's boson image for the Hamiltonian.

2.2.3. Numerical solution of Hill-Wheeler equation with discretization

A numerical solution of the Hill-Wheeler equation (1.3), can be obtained by introducing a discrete set of values α_i ($i = 1,2,\ldots$) for the parameter vector $\alpha = (\alpha^1, \alpha^2, \ldots \alpha^{m_i})$ and by approximating the integral equation by a system of linear equations [26]

$$\sum_j \left[H(\alpha_i,\alpha_j) - EI(\alpha_i,\alpha_j)\right] f(\alpha_j) = 0 \qquad (2.65)$$

We shall restrict ourselves to the subspaces H_Φ of finite dimension d. In that case the system of equations (2.65) is exactly equivalent to the Hill-Wheeler integral equation (1.3) provided the vectors α_i are sufficiently numerous and properly distributed. As a criterium for a good choice of the set α_i, one can check the dimension of the subspace spanned by this set. The dimension d of the subspace H_Φ is equal to the maximum number of non-zero eigenvalues of the overlap matrix $I(\alpha_i,\alpha_j)$ with respect to all possible choices of the set α_i. If the set α_i to be used in the eq. (2.65) gives d non-zero eigenvalues of the overlap matrix $I(\alpha_i,\alpha_j)$ the solution of the eq. (2.65) is formally equivalent to that of eq. (1.3). The expression "formally equivalent" warns that in numerical calculations some information may be lost because of computer round-ups, when the functions $\Phi(x,\alpha_i)$ are not orthogonal enough even if the correct dimension d is reached.

2.2.3.1. The single-parametric GCM

In order to make the numerical solution of the equations (2.65) feasible one tries to replace the parameters α^ν by a single

parameter t (or sometimes few parameters t)

$$\alpha^{\nu} = F_{\nu}(t) \ , \quad \nu = 1,2,\ldots m \qquad (2.66)$$

There are two relevant questions connected with this procedure:

i) Do the functions $\Phi(x,F_{\nu}(t))$still span the complete subspace H_{Φ}? - Answer: This can be always achieved in general: the relation (2.66) represents a curve in the multidimensional space of vectors α and a finite number of points representing d basic vectors α_i, or consequently $\Phi(x,\alpha_i)$, can always be connected by a winding curve.

ii) It is of practical interest whether a set of $\alpha_i = (\alpha_i^1,\alpha_i^2,..\alpha_i^m)$ representing a complete basis can be chosen so that they lie on a simple curve. - This turns out to be possible, but the choice depends on the physical problem considered. For this reason the more concrete procedure for choosing F, eq. (2.66), will be presented in the discussion of quadrupole vibrations, pairing vibrations etc. in chapter 3.

2.2.3.2. A numerical procedure for the single-parametric GCM

The dimension of the subspace H_{Φ} comes out to be large in almost all cases of physical interest, so that a truncation to a smaller subspace H_d is needed for numerical calculations. The following procedure proved useful for the description of low-lying states.

i) Choose $d_1 < d$ and calculate $I_{ij} = \langle\Phi(x,t_i)|\Phi(x,t_j)\rangle$, $i,j = 1,\ldots d_1$; and diagonalize the matrix I_{ij}. The values of t are chosen in a wide enough range around the minimum of $\langle\Phi(x,t_i)|H|\Phi(x,t_i)\rangle/\langle\Phi(x,t_i)|\Phi(x,t_i)\rangle$. Then we test the stability of the results of the diagonalization with respect to the changes in the choice of parameters t_i. If several eigenvalues of I_{ij} are

close to zero one recalculates I_{ij} in a smaller number d_1 of points.

ii) Truncate the subspace H_{d_1} to the subspace H_{d_2} of a dimension $d_2 < d_1$ by rejecting all vectors having a norm a few orders of magnitude smaller than the largest norm.

iii) Diagonalize the Hamiltonian in the subspace H_{d_2}.

The above procedure works if the vectors with small norms represent high energy configurations. In the case where a state with a small norm represents a low energy configuration its intrusion into the subspace of states with large norms can have significant effects. The proper check for such an unexpected difficulty is to allow for a few additional eigenvectors of I and see whether the final spectrum is affected.

Additionally, one may look at all eigenstates Ψ of I having a small norm and check whether $\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$ lies above the interesting low-lying states. Alternatively, one may diagonalize the Hamiltonian within the subspace of small (but not too small) norm and check whether any eigenvalue might be pushed low due to some coherence. If there is an intruder, one should find out a way how to construct it separately and add it to the GC basis $\Phi(x,\alpha)$.

2.3. Current work and open problems

2.3.1. Reduction to families with fewer generator coordinates

In order to reduce the number of generator coordinates one must look at the "energy surface" $E(\alpha^1,\alpha^2,\ldots) = \langle\Phi(\alpha^1,\alpha^2,\ldots)|H|\Phi(\alpha^1,\alpha^2,\ldots)\rangle/\langle\Phi(\alpha^1,\alpha^2,\ldots)|\Phi(\alpha^1,\alpha^2,\ldots)\rangle$. For simplicity, we shall discuss the reduction of a two-parametric family to a one-parametric family.

As a possible criterion, one may choose the points

$(\alpha^1,\alpha^2) \equiv (\alpha,\beta)$ lying on the valley line. This line corresponds to the shallowest ascent from the minimum and therefore to the lowest vibrational frequency, if the states along this line are not too strongly coupled to other "degrees of freedom"*.

The "geography" of the energy surface depends, however, strongly on the choice of the generator coordinates. A change of scale of the generator coordinates can distort the energy surface so that the valley lines get completely changed. The purpose of the present note is to suggest how to choose such a scale that the density of linearly independent states is approximately constant. There is some arbitrariness in defining the density of states. Two procedures will be described using slightly different "definitions" of the density of states.

i) To define the density of linearly independent states we consider the overlap between immediate neighbours only. We expand (assuming Φ to be normalized)

$$I(\alpha\beta,\alpha'\beta') = 1 - g_{11}(\alpha-\alpha')^2 - g_{12}(\alpha-\alpha')(\beta-\beta') - g_{22}(\beta-\beta')^2. \quad (2.67)$$

The matrix $g(\alpha,\beta)$ can be considered as a measure of the density of states, in the sense that for small elements of g neighbouring states have an overlap very close to 1, i.e. are almost linearly dependent.

A constant and isotropic density of states G can be obtained

*The described criterion has been criticized because it ignores the effect of the off-diagonal matrix elements of the Hamiltonian in the GC basis. It has been suggested to take into account the off-diagonal elements at least in the "effective mass" approximation (like in Section 2.2.2.2.). The "effective mass" could largely influence whether it is really the easiest way for a nucleus to vibrate along the valley line or in some other direction. The latter improvement is, however, often impractical because the most time-consuming part of the calculation is to compute just these off-diagonal elements. Once they are calculated one can as well perform a straightforward solution of the Hill-Wheeler equations without reducing the number of parameters.

by a transformation of generator coordinates $u = u(\alpha,\beta)$, $v = v(\alpha,\beta)$, such that

$$I(uv,u'v') = 1 - G\{(u-u')^2 + (v-v')^2\} \approx 1 - G\{u_\alpha^2(\alpha-\alpha')^2 +$$

$$+ u_\alpha u_\beta(\alpha-\alpha')(\beta-\beta') + u_\beta^2(\beta-\beta')^2 + v_\alpha^2(\alpha-\alpha')^2 + v_\alpha v_\beta(\alpha-\alpha')(\beta-\beta') +$$

$$+ v_\beta^2(\beta-\beta')^2\}. \qquad (2.68)$$

Here, $u_\alpha \equiv \partial u/\partial\alpha$ etc. The quantity $G(u,v)$ can be made constant only on a curved surface. It is more practical to make a conformal mapping of the curved surface of generator coordinates onto a plane so as to have $G(u,v)$ depending on position but still being a scalar. The density of states is then locally isotropic but not homogeneous. In this case the energy surface is only conformly distorted and the valley lines do not change.

To get G we compare eqs. (2.67) and (2.68) and the following differential equations have to be solved

$$u_\alpha^2 + v_\alpha^2 = g_{11}/G$$

$$u_\alpha u_\beta + v_\alpha v_\beta = g_{12}/G$$

$$u_\beta^2 + v_\beta^2 = g_{22}/G \ .$$

As there are 3 equations for 3 unknown functions u, v and G a solution should exist with rather general g, at least in the vicinity of the starting point of integration (point of minimum energy).

A simplified and more practical procedure is to make just a linear transformation $u = c_{11}\alpha + c_{12}\beta$, $v = c_{21}\alpha + c_{22}\beta$ so that G is isotropic at the coordinate origin (at the minimum of the energy surface). In the case of "small vibrations" around *one* minimum this will ensure the correct choice of the two normal modes (the shallowest and the steepast ascent). As an illustration see Fig.2.1,

where a distortion of the scale changes completely the valley line. If, however, two or more minima are important a more complicated transformation should be used giving isotropic G at least along the valley line.

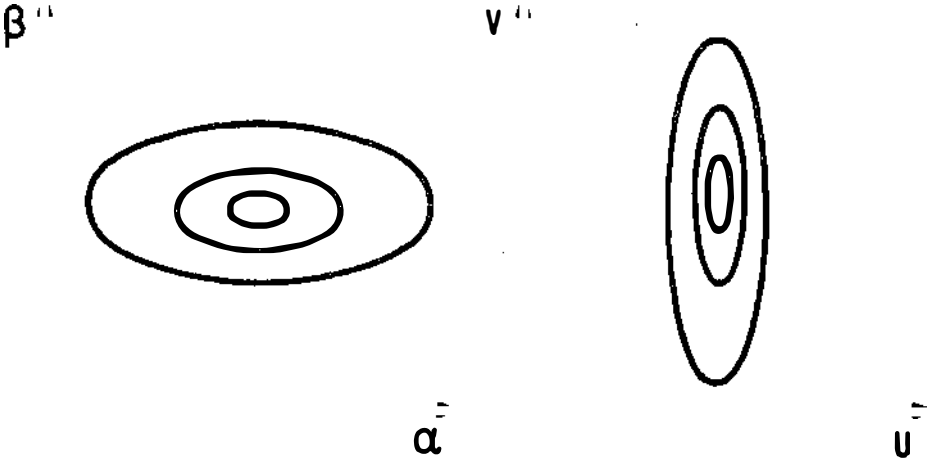

Fig. 2.1.
Lines of equal energy are compared for two different choices of generator coordinates

ii) If the overlaps between neighbouring states were Gaussian, an appropriate metric in the GC space could be defined by choosing as the distance between two points (α_i,β_i) and (α_j,β_j) the expression:

$$d_{ij} = - \ln I(\alpha_i\beta_i,\alpha_j\beta_j).$$

Such a distance would be proportional to the number of linearly independent states between the points i and j.

We use the above definition of d_{ij} even if the overlap is not Gaussian. We start with the minimum point 1 and plot a

neighbouring point 2 at a distance d_{12} from 1. A third point 3 is determined by d_{13}, d_{23}. The position of the fourth point is overdetermined by d_{14}, d_{24}, d_{34}. In practical cases it will be in a certain "error area" given by the intersections of the circles around the points 1,2,3 with radii d_{14}, d_{24}, d_{34} respectively. One proceeds in this way as long as the linear dimensions r_k of the "error area" around k are small compared to the relative distances. One can now calculate the energy surface in a two dimensional plane in which the linearly independent points are isotropic and homogeneous within the "error area" around each point. As soon as the error areas become too large one chooses a new starting point in the direction of shallowest ascent. The above procedure is then repeated. In this way one is able to follow the valley line without plotting the entire GC plane.

2.3.2. Some remarks on complex generator coordinates

A complex generator coordinate can be introduced in two ways:

a) One generates a one-parametric family $\Phi(x;\alpha)$ along a chosen line or contour c in the complex plane α (see section 2.2.2.2) One has $\Psi(x) = \int_c f(\alpha)\, \Phi(x;\alpha)d\alpha$.

b) One generates a two-parametric family with $Re\alpha$ and $Im\alpha$ as independent generator coordinates. Then

$$\Psi(x) = \iint f(\alpha)\Phi(x;\alpha)dRe\alpha dIm\alpha$$

like in section 2.2.1.

The purpose of introducing a complex generator coordinate may be the following

i) For real α, the solution of Hill-Wheeler equation may give for $f(\alpha)$ a distribution (see sections 1.1. and 2.2.1) while the extension of α into the complex plane may allow to restrict ourselves

to an analytic function $f(\alpha)$. There is a theorem* that any distribution f can be written as a limiting value of two analytic functions F on the real axis: $f(t) = F_1(t+i0) - F_2(t-i0)$. Here F_1 is regular in the entire upper half-plane and (highly) singular in the lower half-plane of the complex plane while F_2 behaves vice versa. If the generator function Φ is regular near the real axis one can shift the path of integration from the awkward vicinity of the real axis to any convenient contour c. One can write

$$\Psi(x) = \int_{-\infty}^{\infty} f(t)\Phi(x;t)dt = \int_{c \text{ (in upper half-plane)}} \{F_1(\alpha)\Phi(x;\alpha) - F_2(\alpha^*)\Phi(x;\alpha^*)\}d\alpha.$$

ii) As is shown in ref. [2] for the case of GOA, $\mathrm{Im}\alpha$ can be interpreted as a conjugate variable to $\mathrm{Re}\alpha$ (like momentum versus position). In Section 2.2.2.2. the phase change in α was exploited to make $\mathrm{Re}\alpha e^{i\phi}$ and $\mathrm{Im}\alpha e^{i\phi}$ resemble as much as possible the position and momentum of an anharmonic oscillator (so that the Hamiltonian $\hat{h}$ is quadratic in the "momentum"). It is an open question whether $\mathrm{Im}\alpha$ can be interpreted as a conjugate generator coordinate for a more general generator coordinate family. What does such a conjugate generator coordinate mean physically? What is the underlying collective dynamical variable?

iii) From the practical point of view, more experience is needed to see in which cases $\mathrm{Im}\alpha$ generates a useful and important part of the Hilbert space. It is an open question whether the one-parametric version a) is already a good extension of the real generator parameter due to the fact that $\Phi(x;\alpha)$ is not a general function of two generator coordinates $\mathrm{Re}\alpha$ and $\mathrm{Im}\alpha$ but it is an analytic func function. Also, it is an open question how to choose the optimal contour c; if $\Phi(x;\alpha)$ is a regular function, the value of the integral does not depend on the integration path in principle, however, the numerical truncations and round-offs can be quite different.

*see for example B.W.Roos, Analytic Functions and Distributions in Physics and Engineering (John Wiley, New York, 1969).

3. BOUND STATES

3.1. Successes and some difficulties of methods commonly used to describe nuclear bound states

3.1.1. Projected Hartree-Fock (PHF) and α-particle model calculations in 1d2s-nuclei

During the last ten years, there has been considerable progress in understanding the structure of light nuclei. In 1p shell nuclei and the first half of 1d2s-shell both PHF and α-particle model were fairly successeful, while in the second half of 1d2s-shell the success has been meagre. PHF calculations and α-model calculations have solved some outstanding old problems like the enhancement of E2-matrix elements and the occurrence at low energy of non-normal parity and intruder states. Nevertheless, many problems still remain and it is worthwhile to find better methods to treat a finite fermion system. One such method might be the GCM.

We first want to review some of the problems encountered in PHF calculations. For computational reasons, most of the PHF calculations have been done with central forces only, restricting the wave function to be an eigenfunction of L^2 and S^2 and belonging to the most symmetric partition $[f]$. So one can expect that some of the difficulties are due to this restriction and will probably disappear if spin-exchange and noncentral forces are used to mix states of different symmetry. In this case the final wavefunctions do no longer have the form of a projected Slater determinant but become more related to the intermediate coupling wave-functions of Kurath. From his early work we may expect that the too low excitation energy of the first 2^+ state in even-even nuclei will improve. Also, the occurrence of the lowest K = 2, L = 2 level at too low energy in nuclei like ^{10}Be, ^{16}O or ^{24}Mg is

believed to be due to the neglect of non-central forces. It is easy to study the effect of forces breaking the SU (4) symmetry in a simple way using a one-body $l.s$ force to mix states belonging to different partitions. This is presently being done in Mol.

An alternative way is to change the single particle basis to include $l.s$ splitting and the relative shift of 2s- to 1d-single particle energies (see also Ch. 3.3.2).

Another systematic deviation between experiment and PHF predictions is the diffraction dip in the elastic form factor at large momentum transfer. Although PHF calculations improve the elastic form factor substantially in nuclei having a ground state quadrupole moment different from zero (like ^{9}Be), the diffraction dip at $q^2 \approx 10$ fm^{-2} has not been reproduced. A GCM approach, treating the oscillator size parameter as generator coordinate, might possibly correct for this discrepancy as indicated by a preliminary calculation for ^{4}He in Ljubljana.

In most PHF calculations done so far, the structure of the intrinsic state is guessed, either from standard HF results or from the SU(3) model, and the expectation value of the Hamiltonian is minimized with respect to several variational parameters. As soon as one tries to describe excited states which do not belong to the ground state band, one gets into the difficulty of guessing the intrinsic state for these. For different excited states, different variational parameters may be needed and this choice rests at present on physical intuition. For example, for describing the 3^- state in ^{12}C, one may expect that an octupole deformation may be more useful than a quadrupole deformation, but what parameters should one choose to describe e.g. a 1^+ state? We are lacking a more systematic way how to obtain a good variational function for excited states. There is, however, another difficulty in PHF. States of equal J, but projected from different intrinsic states, are in general non-orthogonal. (In GCM they are mixed and they are automatically orthogonal).

In nuclei with rotation-like spectra like ^{20}Ne or ^{24}Mg, the moment of inertia is experimentally found to increase gradually with angular momentum, while in PHF calculations, it remains almost constant. Is this an effect of pairing, which so far was believed not to be important for N = Z nuclei?

Apart from these rather general problems, there are some special difficulties in the 17 < A < 19 region. Whereas in nuclei up to ^{12}C, E2 matrix elements are generally obtained in agreement or even larger than the experimental value, the quadrupole moment of ^{17}O calculated with the rather elaborate PHF wave function is only half the experimental value. Also, the odd-parity levels in ^{17}O or ^{19}F remain too high (both 1p - 1h or 3p - 3h) and the 2p - 2h state in ^{18}O does not come down sufficiently. Does this mean that these heavier nuclei require us to take some other degree of freedom into account or may this be related in some way to admixtures of the 4p - 4h states in ^{16}O (which also remains an unsolved problem)?

In contrast to the results of extensive Hartree-Fock calculations in a large single particle space, the results in the Margenau-Brink α-model are easy to visualize. This certainly is an important advantage of the α-model as it may suggest some simple kind of vibrational excitations (see the application of GCM to the α-model wave functions in Sec.3.2.3). Apart from this simplicity of picture (e.g. the complicated 8p - 8h state in ^{16}O in a central potential being replaced by four α-particles in a line), there are forces (e.g. the B1 force [29]), for which the α-model constitutes an improvement over the restricted HF calculations at least for the Z = N even nuclei up to ^{20}Ne. This improvement shows up in an increase in binding energy, which is due to the fact that the α-model wave functions are not truncated to a finite subspace of Hilbert space and that several symmetries in the intrinsic state (parity and axial symmetry) are given up. Giving up the parity has as a happy consequence that states of

negative parity (3^- states in ^{12}C and ^{16}O) are described by the same configuration of α-clusters as the ground state. The basis of functions used in the α-model (i.e. different wells around different points in space) should probably also allow a simpler description of α-decay than the usual restricted HF basis.

Apart from this success of the α-model for nuclei with $A \leq 20$, the model is found to be less good for the heavier nuclei than restricted HF calculations. Smaller binding energies are obtained. In ^{24}Mg and ^{28}Si, the α-model gives the wrong sign for the deformation. For these heavier nuclei, the problem of guessing a good configuration of α-clusters, if any, becomes very important as the number of parameters increases very rapidly. This is an important point since calculations with projected states in lighter nuclei have shown that the most stable configuration does not necessarily correspond to a configuration with high symmetry.

A common difficulty to PHF and α-model calculations is the mixing of different intrinsic states in order to describe the experimental interband transitions. In nuclei like ^{12}C or ^{16}O, the α-model suggests an easy way to obtain mixing by gradually changing the α-configuration from one state to the other. The GCM is a way to describe the mixing of different configurations (see Sec. 3.2.3).

To conclude this short review of PHF and α-model calculations, we want to stress the importance of the nuclear interaction used. The quoted difficulties must be interpreted as those that remain when a "generally good" force is being used. It may be that some of the difficulties disappear when a "better" force is used, but probably other new difficulties would appear at the same time.

3.1.2. Angular momentum projected Hartree-Bogoljubov theory

In HFP calculations (HF-model with angular momentum projection after variation) the energies in the ground state rotational bands of light nuclei strongly depend on the effective force used. Nevertheless, it is a common feature of all existing HFP spectra, even those calculated with noncentral forces and symmetry breaking wave functions in large basis spaces, that they are clearly compressed compared to experimental values and that they do not properly reproduce the increase of the experimental moments of inertia with increasing J-value [17]. This seems to be a weakness of the HF model itself and therefore it is senseful to go beyond the HF picture (a single Slater determinant). Apart from the methods listed in Sec.3.2, 3.3, there is one way to do this, namely to include pairing correlations by the Hartree-Bogoljubov (HB) method. [19]. In all nuclei of the 1d2s-shell the HB procedure yields solutions with more than 1.5 MeV pairing energy; only ^{20}Ne, ^{24}Mg (triaxial), ^{28}Si and ^{32}S (triaxial) reduce to pure HF solutions. (For the description of nuclei with N = Z one has to take into account pairing correlation with T=0). In the cranking formalism the paired solutions generally show a markedly smaller moment of inertia than the HF solution. In all paired wavefunctions, projection of angular momentum and particle number after the variation (HBP) yields generally an increase [18] of the excitation energies of the ground state rotational band up to 100 % compared to HFP. The agreement of excitation energies with experiment and in some cases also the J-dependence of the moments of inertia are improved. The quadrupole moments of the rotational states show a little antistretching effect. There are indications that, in contrast to HF, angular momentum projection before the variation (PHB) is necessary even for strongly deformed light nuclei. This has been performed approximately in the framework of a constrained HB theory (CHB) with the "pairing energy" Δ as the constrained quantity [33]. In this method one defines the intrinsic state for

each J by minimizing the binding energy $E_J(\Delta)$ in dependence of Δ. It turns out that the minima lie at quite different positions indicating a marked change of the intrinsic wavefunction with J. This change is in general larger than found in a PHF procedure. The PHB method approximated by CHB shows a strong antipairing effect with increasing J and a phase transition into the HFP state at about $J = 4^+$ or $J = 6^+$ as calculation in ^{22}Ne, ^{24}Ne and ^{30}Si indicate. Due to this, the experimental increase of the moments of inertia with increasing angular momentum is reproduced with much better agreement than in PHF and HBP. In these results the antistretching effect can no longer be recognized since the higher J-levels prefer unpaired intrinsic states with larger quadrupole moments.

There are some difficulties and shortcomings encountered in HBP and CHB:

(i) Since the CHB method yields markedly different intrinsic states for the different J-levels, correct angular momentum projection before the HB variation seems to be necessary. This has been formulated theoretically, but explicit realistic calculations are missing. (ii) It is a general feature of all variational techniques, that variation with projected wavefunctions favours the symmetry breaking part of the intrinsic wavefunction. So one might expect even for ^{20}Ne, ^{24}Mg (triaxial), ^{28}Si and ^{32}S (triaxial) a little amount of pairing as soon as one varies with particle number projected wavefunctions. (iii) Up to now there is to our knowledge no proper attempt to investigate the effect of pairing correlations in excited states of light nuclei, which do not belong to the ground state rotational band. Especially for nuclei with pairing correlations in the ground state this would be interesting. (iv) Nuclei like ^{24}Ne or ^{32}S show a vibrational rather than a rotational spectrum. Their intrinsic states are probably not well described by a single wavefunction of HB-type.

It is hoped that some of difficulties in (iii) and (iv) will be resolved by the GCM, for example by using a two-parametric

generator function $\Phi(x,\beta,\Delta)$, where β and Δ are related to the deformation and the pairing degree of freedom. (see Section 3.3.4).

3.2. *Beyond Hartree-Fock, α-particle model and Hartree-Bogoljubov theory. - The generator coordinate method, Present status.*

3.2.1. Introduction

There are several ways in which the GCM could improve on the HF and HB results, and which are feasible with presently existing computer programs. The essential condition for being able to carry out a GCM calculation in practice is to have a generator wave function which is simple enough: the only cases considered so far are restricted to using one or a few Slater determinants, angular momentum projected Slater-determinants or N-projected BCS functions.

The choice of generator function is usually based on physical intuition and may depend on the particular state under consideration. For example, one choose as a generator function a particular combination of Slater determinants of single particle functions in a potential whose shape changes in the required way. This is e.q. the case if one takes the class of Nilsson functions, treating the deformation of the oscillator potential as generator coordinate to describe quadrupole vibrations. Another example is in obtaining the generator functions from a constrained Hartree-Fock calculation, where the constrained physical quantity is the one belonging in a most typical way to the nuclear motion under consideration.For example, in the case of quadrupole vibrations, one would carry out a HF calculation where the quadrupole moment is constrained.

The application of the GCM started chronologically with Gaussian overlay approximation. We review results of those applications in Section 3.2.2. The calculations based on the α-particle model determinant as a generator function were performed next. The trial function obtained by projecting angular momentum

from a combination of different α-particle configurations provided a rather good spectrum of ^{12}C (Section 3.2.3). The description of seniority zero states (pairing vibrational states) was based on the N-projected BCS as the generator function (Section 3.2.5). A description of light nuclei based on deformed determinants as generator functions required much more effort due to quite complicated projection of angular momentum. Only one result based on the latter generator function was published untill now (Section 3.2.4).

3.2.2. Gaussian overlap approximation

The following calculations have been done by using the Gaussian overlap approximation described in Sec.2.2.1.:

1. Griffin calculated [7] two excited states of ^{16}O, the second 0^+ and the first 2^+ state. He supposed the 0^+ state to be a dilatational collective state and took as the generator function the lowest harmonic oscillator Slater determinant. The generator coordinate was a scale factor: $x_j = x'_j e^{-\alpha}$; $y_j = y'_j e^{-\alpha}$, $z_j = z'_j e^{-\alpha}$, where x'_j, y'_j, z'_j, x_j, y_j, z_j are single particle coordinates. He got too high energy for a factor of more than two and also the matrix element for the transition to the ground 0^+ state was too large. His suggestion was that enlarging the basis by including two particle-two hole states would improve the results.

   For the description of the 2^+ state he used as the generator coordinate the deformation parameter β defined by: $x_j = x'_j e^{\beta}$; $y_j = y'_j e^{\beta}$; $z_j = z'_j e^{-2\beta}$. He got similar results as for 0^+ state: too high energy, too large matrix element for the transition to the ground 0^+ state.

2. Bar-Touv [20] used the Slater determinants $\Phi(x,q)$ of the constrained Hartree-Fock calculation as the generator functions. The constrained quantity was the expectation value q of the

mass quadrupole moment Q_{20}. In the study of the excited 0^+ state in ^{20}Ne, the following restrictions were imposed: inert ^{16}O core, single particle basis limited to the 1d2s space, axial symmetry, fourfold degeneracy.

As the residual interaction a Yukawa force with Rosenfeld mixture was used. Bar-Touv did not solve the corresponding Hill-Wheeler equation, but identified the intrinsic function of the first vibrational state with the first derivative of $\Phi(x,q)$ (as in the Gaussian overlap approximation)

$$\Phi_{excited} = \text{const.} \left[\partial\Phi(x,q)/\partial q\right]_{q=q_0} \qquad (3.1)$$

The energy of this state is 6.9 MeV and it is 1 MeV below the Tamm-Dancoff solution; the overlap of the two functions is almost complete.

The curve $E_{HF}(q)$ (Fig.3.1 in ref.[20]) has, however, another minimum at 6.4 MeV above the ground state minimum, so the stability of the solution (3.1) has to be tested by a more extended generator coordinate calculation which includes the anharmonicity of the "potential" $E_{HF}(q)$ and the proper nondiagonal elements. It is difficult to compare this result and results of Secs.3.2.4. and 3.3.1, because different generator coordinate functions and parameters have been used.

3. Cluster vibrations in the GC-method.

Cluster vibrations were described in the GCM starting from the alpha particle model of Brink. In this model one introduces antisymmetrized many-body wave functions $\Phi(x,b,R_i)$ which depend on all particle coordinates x and on a set of parameters, viz. the mean positions R_i of the clusters and their radius b. Using these functions as generating functions of the Hill-Wheeler method, one can describe oscillations of cluster configurations. For practical work, "normal parameters"

are introduced in the following way: Adopting a certain point symmetry for the equilibrium configuration of clusters and minimizing the expectation value of the Hamiltonian H in the state $\Phi(x,b,R_i)$ with respect to b and R_i, we are left with a set of equilibrium parameters R_i^o. The differences $\delta R_i = R_i - R_i^o$ are then combined to form "normal parameters" q_μ according to the underlying point symmetry.

Using the Gaussian overlap approximation, the Hill-Wheeler problem is equivalent to solving a set of RPA-like equations(2.12) whose dimension equals twice the number of parameters [2]. The matrices A and B are essentially determined by the matrix elements

$$\langle \partial/\partial q_\mu \; \Phi(x,R_i) | H | \partial/\partial q_\nu \; \Phi(x,R_i) \rangle_{q_\mu = q_\nu = o}$$

and

$$\langle \Phi(x,R_i) | H | \partial/\partial q_\mu \partial q_\nu \; \Phi(x,R_i) \rangle_{q_\mu = q_\nu = o}$$

respectively. Numerical calculations can be simplified considerably by making full use of the symmetry properties of the underlying point group [2].

The procedure as outlined above has been carried out numerically for ^{20}Ne with D_{3h} - symmetry (trigonal bipyramid) using as two-body interaction the Brink-Boeker force B1. The vibrational energies E turned out to be rather high [2], apart from the octupole mode with an excitation energy of 4.4 MeV. This mode may be identified as the intrinsic state for the observed $1^-, 3^-, 5^-, \ldots$ rotational band at 5,8 MeV.

3.2.3. Mixing of α-particle configurations in ^{12}C

There have been two attempts to describe the low lying states in ^{12}C by the generator coordinate method:

(1) Friedrich, Satpathy and Weiguny [22] (see also ref. [23]) used as generator functions the intrinsic wave functions

$$\Phi^{+}(x,\Theta) = \Phi(x,\Theta,d) + \Phi(x,\pi+\Theta,d)$$

for arbitrary triangular configurations as in Fig. 3.1.

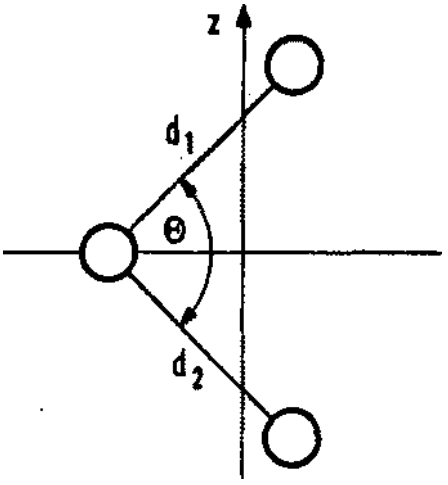

Fig. 3.1. An arbitrary triangular configuration for ^{12}C. The origin is at the centre of clusters defined by $\sum_i R_i = 0$.

The generator coordinate parameter was the angle Θ, while $d_1 = d_2 = d$ was determined variationally for $\Theta_{min} = 60^{\circ}$.

The Hill-Wheeler equation was solved approximately by choosing six points for the parameter Θ.

The two lowest solutions $\Psi_\nu = \sum_i C_{\nu i}\Phi^{+}(x,\Theta_i)$, $\nu = 1,2$, were analysed by calculating the probabilities $w_\nu(\Theta_i) = |\langle\Phi^{+}(\Theta_i)|\Psi_\nu\rangle|^2$. The result showed that for the lowest solution Ψ_1 the probability $w_1(60^{\circ}) = 0.91$. The excited state Ψ_2 had the largest overlap with the $\Phi^{+}(x,150^{\circ})$ configuration and not with the linear chain ($\Theta = 180^{\circ}$).

The result of this calculation looked like a confirmation

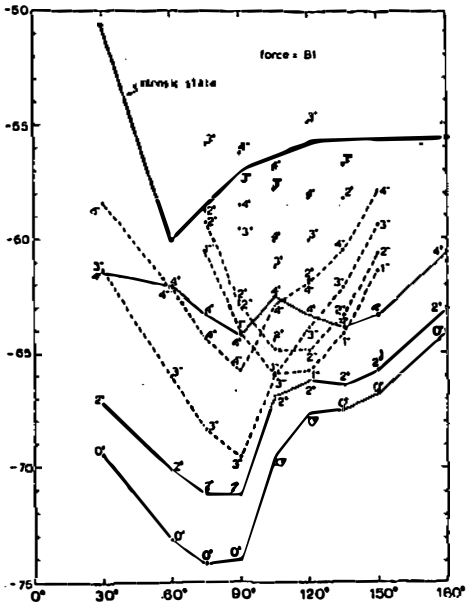

Fig. 3.2 The energies of angular-momentum-projected states calculated with the Brink and Boeker B1 potential as a function of hinge angle θ. Ref.[24].

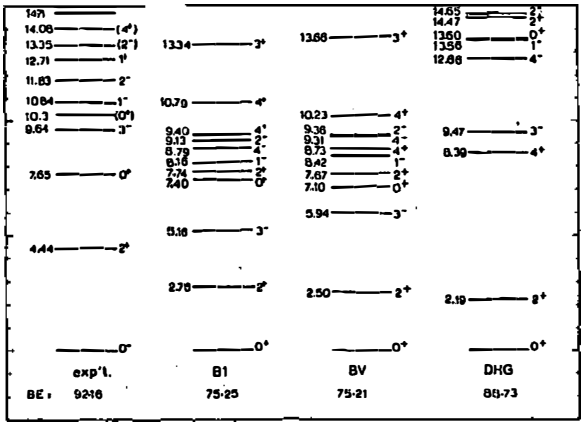

Fig. 3.3 The energy levels of ^{12}C obtained by a Hill-Wheeler projection over the hinge angle with forces B1, BV and DHG (see text). The absolute binding energies are given in the bottom line and the experimental results are shown for comparison. Ref.[24].

of the picture that the ground state is an oblate state and the second 0^+ corresponds to one strongly deformed prolate intrinsic state. This picture will be somewhat "corrected" using angular momentum projected states.

(2) De Takacsy [9] used as intrinsic function a Slater determinant $\Phi(x,d,\Theta)$ corresponding to an arbitrary triangle configuration shown in Fig.3.1. The restriction $d_1=d_2=d$ was imposed. As generator functions, states of good angular momentum and good parity projected from the intrinsic state, are used;

$$\Phi_{JM}(x,d,\Theta) = \frac{2J+1}{8\pi^2} \int d\Omega\, D^{J*}_{MK}(\Omega)\, R(\Omega)\, \Phi(x,d,\Theta)\,.$$

The energies of such angular-momentum projected configurations are compared with the energy of the intrinsic states $\Phi(x,d,\Theta)$in Fig.3.2.The energy of the ground state $E^{0^+}(\Theta)$, has its minimum around 75^o and not at 60^o as for the intrinsic state.

The Hill-Wheeler equation was diagonalized approximately using the subspace spanned by 6 values of Θ_i.

The result is shown in Fig.3.3. This provided candidates in the right energy region for most of the experimental states in ^{12}C and the information that some of the states (e.g. 1^+ state at 12,7 MeV) are not in the subspace spanned by an α-particle model wave function. In addition, a different generator function would be needed for describing the moment of inertia parameter.

3.2.4. Deformed determinants of the 1d2s single particle wave functions as generator functions - small space, no symmetry restriction

Instead of using a generator function of high symmetry (Secs. 3.2.3, 3.3.1), one may obtain generator functions $\Phi^J(x,\alpha)$ by projecting angular momentum from a Slater determinant built from single particle functions $\Phi_n(x,\alpha)$ which are general linear

combinations of single particle shell model functions within one (or two) shells. The parameter α either describes the shape of the single-particle potential or represents the expectation value of a certain one-body operator, e.g. the quadrupole moment Q_{20}.

The single particle wave functions ϕ_n *either* depend on the shape of the nucleus through the (Nilsson-like) coefficients $C_{nj}(\alpha)$

$$\phi_n(x,\alpha) = \sum_{j=1}^{L} C_{nj}(\alpha)\, \psi_j(x) \quad , \quad n = 1,2,\ldots N$$

where $\psi_j(x)$ are for example, the harmonic-oscillator functions, *or* $\phi_n(x,\alpha)$ are constrained Hartree-Fock solutions. Till now, for technical reasons, axially symmetric functions ϕ_n were used only.

In both cases the Hill-Wheeler equation is

$$\sum_{\beta} \langle \alpha JM|H|\beta JM\rangle - E_J \langle \alpha JM|\beta JM\rangle\, f^J_\beta = 0 \qquad (3.2)$$

where $|\alpha JM\rangle$ is a state obtained by projecting angular momentum from an axially symmetric state $\Phi_M(x,\alpha)$. The central problem in solving the Hill-Wheeler equation is the calculation of the matrix elements

$$H^J_{\alpha\beta} \equiv \langle \alpha JM|H|\beta JM\rangle \quad \text{and} \quad I^J_{\alpha\beta} \equiv \langle \alpha JM|\beta JM\rangle \, .$$

Mihailović, Kujawski and Lesjak ([25]) used as generator function a Slater determinant of Nilsson's single particle functions and treated the deformation parameter η as GC parameter. In an illustrative study of low-lying states in ^{20}Ne, the generator coordinate function is approximated by an inert ^{16}O core and four particles in the Nilsson orbital No.6 ($k = \pm 1/2$) which contains the j orbitals $d_{5/2}$, $d_{3/2}$, $2s_{1/2}$.

As effective nuclear interaction the force proposed by Rosenfeld has been used.

The Hill-Wheeler equation is solved approximately in the subspace spanned by 5 points. The solution provided 1 to 2 sensible states for each $J = 0^+, 2^+, 4^+, 6^+$. The lowest solutions for each J are "interpreted" as the rotation band. The dependence E(J) was improved compared to HF.

3.2.5. Pairing vibrations

Properties of states which are strongly excited by two-nucleon transfer reactions with J = 0, T = 1 are described in a-part of the seniority-zero subspace which may be spanned by the N-projected BCS function depending on the gap parameter Δ. In the calculation of Justin, Mihailović and Rosina [26] the following trial function has been used

$$\Psi(x) = \int f(\Delta)\Phi^{N}_{BCS}(x;\Delta,\lambda)d\Delta \qquad (3.3)$$

In the trial function (3.3) the simple BCS dependence on the parameter Δ was chosen and for each Δ the parameter λ is fixed by the constraint $\langle\hat{N}\rangle = N$. This is a poor approximation [26,27] for closed shell nuclei because some important two-quasiparticle configurations appear with a too small norm. To avoid this trouble one may use λ as the second generator coordinate, or, what Siegal and Sorensen did [27], introduce the trial function of the form

$$\Psi(x) = \int f_1(\Delta)\Phi^{N}_{BCS}(x;\Delta,\lambda)d\Delta + \int f_2(\Delta)\tilde{\Phi}^{N}_{BCS}(x;\Delta,\lambda_<,\lambda_>)d\Delta, \qquad (3.4)$$

Here λ is fixed by the constraint $\langle\hat{N}\rangle = N$ and the values of the parameters $\lambda_<$ and $\lambda_>$ are chosen so that for single particle levels below the Fermi surface $\lambda_<$ corresponds to $\langle\hat{N}\rangle = N-2$ and for those above the Fermi surface $\lambda_>$ corresponds to $\langle\hat{N}\rangle = N+2$.

The Hill-Wheeler equation was solved approximately by diagonalization in a small part of seniority zero subspace spanned

Table 1. Energies E of first excited 0^+ state and ratios of transition rates for (t, p) reaction $R_{t,p} = \left[\frac{\langle pv(N+2)|\sum_\alpha A_\alpha a^+_{\alpha m} a^+_{\alpha -m}|g(N)\rangle}{\langle g(N+2)|\sum_\alpha A_\alpha a^+_{\alpha m} a^+_{\alpha -m}|g(N)\rangle}\right]^2$ for Sn isotopes. (Ref. 26).

A		114		116		118		120		122		124	
		E(MeV)	$R_{t,p}$	E(MeV)	$R_{t,p}$	E(MeV)	$R_{t,p}$	E(MeV)	$R_{t,p}$	E(MeV)	$R_{t,p}$	E(MeV)	$R_{t,p}$
Exp.		2.16	0.10	1.8		2.06	0.015	2.15	0.015			2.3	0.07
		1.45	0.07	1.6		1.76	0.015	1.88	0.015				
N–proj. 5 s.p.l. $G_1(A)$		2.08	0.19	2.11	0.06	2.53	0.005	2.17	0.005	2.56	1.10^{-4}	2.58	1.10^{-5}
Appr. N–proj. 5 s.p.l. $G_1(A)$	$A_\alpha^{(1)}$	2.06	0.14	2.18	0.056	2.51	0.02	2.78	0.007	2.25	0.001	2.60	3.10^{-4}
	$A_\alpha^{(2)}$		0.17		0.02		0.001		0.003		0.024		0.02
	$A_\alpha^{(3)}$		0.11		0.005		0.005		0.003		0.03		0.03
Appr. N–proj. 16 s.p.l. $G_1(A)$	$A_\alpha^{(1)}$	4.62	0.10	4.52	0.05	4.82	0.06	4.84	0.05	5.07	0.046	5.37	0.05
	$A_\alpha^{(2)}$		0.09		0.15		0.016		0.014		0.016		0.03
	$A_\alpha^{(3)}$		0.08		0.03		0.024		0.012		0.013		0.03
Appr. N–proj. 16 s.p.l. $G_2(A)$	$A_\alpha^{(1)}$	2.48	0.14	2.01	0.91	1.85	0.42	1.19	0.38	1.97	0.082	2.92	0.08
	$A_\alpha^{(2)}$		0.02		0.14		0.015		0.033		0.047		0.10
	$A_\alpha^{(3)}$		0.08		0.08		1.10^{-4}		0.006		0.03		0.03

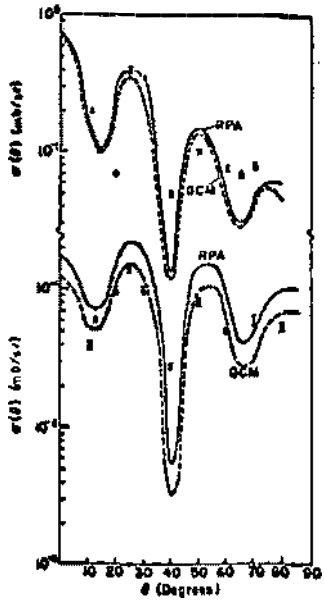

Fig. 4.4 Top: comparison of wave function (3.4), RPA and experimental data (for references, see ref.[27]) for $^{206}Pb(t,p)$ ^{208}Pb; theoretical curves use DWBA code TWOPAR. The GCM ground state uses 8 levels; G = 0.125; Q = 5.628 MeV. Incident energy = 20 MeV.

Bottom: comparison of wave function (3.4), RPA and data for excited 0^+ state for ^{206}Pb (t,p) ^{208}Pb .

GCM uses 13 levels, G = 0.096; Q = 0.757 MeV. Incident energy = 20 MeV. Ref.[27].

Table 2

Comparison of DWBA average differential cross sections using 2-λ GCM and RPA [8]) wave functions with experimental results of ref. [18])

Cross section	Expt. (mb/sr)	GCM (mb/sr)	RPA (mb/sr)
$\bar{\sigma}_A(^{206}Pb(t,p)^{208}Pb(DPV))$	0.053	0.081	0.113
$\bar{\sigma}_B(^{208}Pb(t,p)^{210}Pb)$	0.058	0.126	0.110
$\bar{\sigma}_{B'}(^{210}Pb(p,t)^{208}Pb)$	0.116	0.131	0.097
$\bar{\sigma}_C(^{208}Pb(p,t)^{206}Pb)$	0.11	0.120	0.100
$\bar{\sigma}_{C'}(^{206}Pb(t,p)^{208}Pb)$	0.135	0.198	0.216
$\bar{\sigma}_D(^{210}Pb(p,t)^{208}Pb(DPV))$	0.14	0.090	0.134

Normalizations are 310 for (t, p) and 110 for (p, t). (Ref. 27).

by generator functions corresponding to between five and ten values of the parameter Δ_i.

The method based on (3.3) and (3.4) was used to study pairing vibrational states in Ni, Sn and Pb isotopes. So far, as the residual force, the pairing force with constant matrix elements was used in all calculations.

The quality of results of the calculations are illustrated in Table 1 for Sn isotopes and Fig.3.4. and Table 2 for Pb isotopes. One may say that even with a schematic interaction a fair agreement with experiment is obtained for the energies of 0^+ states and the transfer cross section.

3.3. Work in progress and open problems

3.3.1. "Breathing" and "quadrupole" vibrations

Caurier, Bourotte-Bilwes and Abgrall [28] started with single particle wave functions of a deformed harmonic oscillator potential $V(b,\beta) = \hbar^2/2Mb^4\ (x^2+y^2)e^{-\beta}+z^2e^{2\beta}$ which depends on the size parameter b and the deformation parameter β. They filled the lowest single particle levels in a way suggested by SU (3) and obtained a Slater determinant $\Phi(x,b,\beta)$ belonging to the most symmetric partition $[f]$. Then they made the wave function translation invariant and they used the angular momentum J-projected function $\Phi_J(x,b,\beta) = P^J\Phi(x,b,\beta)$ as the generator function,

$$\Psi_J(x) = \int\int f(b,\beta)\Phi_J(x,b,\beta)db\ d\beta\ .$$

Three different calculations were performed: (i) "breathing" mode: $f(b,\beta) = f(b)\delta(\beta-\beta_o)$ where β_o is the deformation of the Hartree-Fock minimum, (ii) "quadrupole" vibrations: $f(b,\beta) = f(\beta)\delta(b-b_o)$ where b_o is the value of the size parameter at the Hartree-Fock minimum, (iii) "coupled vibrations" where $f(b,\beta)$ is unrestricted.

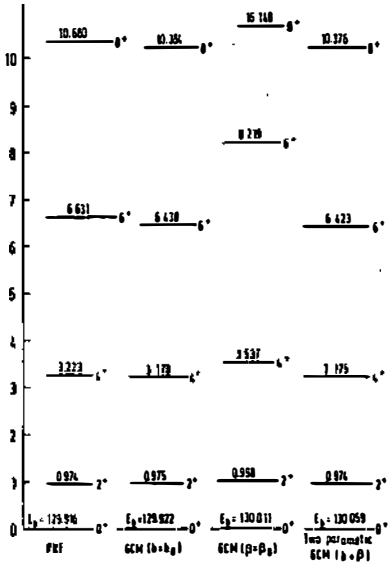

Fig. 3.5a Ground state rotational band of ^{20}Ne. Ref.[28].

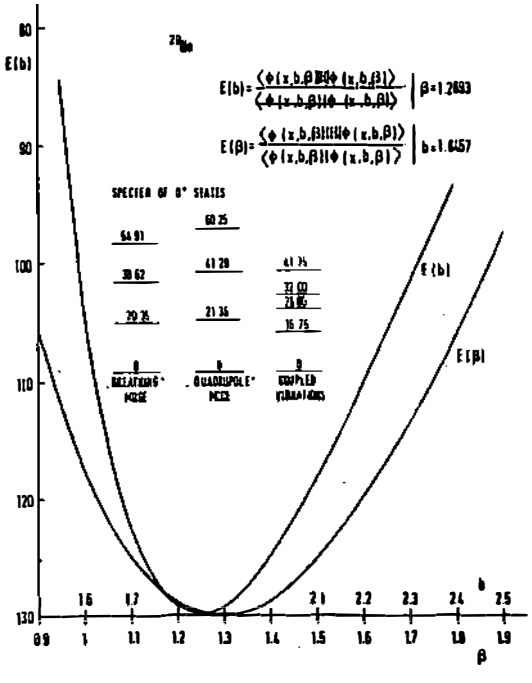

Fig. 3.5b Energy curves and spectrum of 0^+ states. Ref.[28].

As an effective nuclear interaction the force proposed by Brink and Boeker [29] was used.

The Hill-Wheeler equation was solved by choosing a few points for the parameters b and β.

This work is partly a numerical experiment and partly a search to see if given degrees of freedom span a subspace suitable for describing low lying states. The results show that the ground state and its rotational band are not affected by the new degrees of freedom (Fig.3.5a). A different generator function will be needed to improve the rotational spectrum. On the other hand the additional degree of freedom has a large effect on excited states; the results in Fig.3.5b show that the excited 0^+ states are quite different depending on whether one allows one or both degrees of freedom.

Immediately after the Seminar devoted to the GCM, Caurier calculated the "breathing" and "quadrupole" states in ^{16}O using the generator function of the same symmetry as in the calculation of ^{20}Ne. Let us note that the 6,06 MeV 0^+ states in ^{16}O does not belong to this "breathing and quadrupole" subspace.

3.3.2. A two-parametric generator function for 1d2s nuclei

A more complete calculation (which has not yet been performed) would introduce the two-parametric generator functions $\Phi^J(x,\eta,\varepsilon)$ by projecting angular momentum from a Slater determinant of Nilsson single particle functions. The two parameters $\eta=\beta/C$ and $\varepsilon=D/C$ are defined through the Nilsson potential

$$h_{Nilsson} = h_{spher.} + \beta r^2 Y_{20} + C\, \ell.s + D\ell^2 .$$

The parameter η describes the degree of the deformation compared to the degree of the $\ell.s$ coupling, while the parameter ε

refers to the relative amplitudes of 1d to 2s states. The relevance of the latter parameter is supported by Zuker's automatic shell model calculation [30] where, even in a very large basis, the single particle energies ε_{1d} and ε_{2s} have to be used as fitting parameters.

A calculation based on generator functions $\Phi^J(x,\eta,\varepsilon)$ is now in progress in Ljubljana.

3.3.3. Mixing of different generator coordinate families

The following function

$$\Psi^J(x) = \int \sum_k f_k^J(\alpha)\, P^J\, \Phi_k(x,\alpha) \qquad (3.5)$$

represents a generalization of the cases described in Secs. 3.2.4. and 3.3.2. The functions Φ_k are different intrinsic determinants (e.g. 0p-0h, 1p-1h, ... np-nh configurations). Here one uses two degrees of freedom, summing over α and over k, in order to get an appropriate trial function. Both degrees are unnecessary if one takes large enough number of configurations Φ_k, but the idea is to take a small number (two or three) of them and to "complete" the basis by taking α as a generator coordinate.

The diagonalization of the Hamiltonian in the subspace spanned by the functions (3.5) is equivalent to solving the system of coupled Hill-Wheeler equations. By introducing a discrete set of values for the parameter α, one gets a set of coupled linear equations similar to eq. (3.2) except that an additional index k for different configurations is needed,

$$\sum_{(k'\beta)} \{\langle(k\alpha)JM|H|(k'\beta)JM\rangle - E_J\langle(k\alpha)JM|(k'\beta)JM\rangle\} f^J_{(k'\beta)} = 0 \ .$$

The choice of the configurations Φ_k depends on the problem. Good candidates for the description of low lying states of even J in the

second half of 1d2s shell are 0p-0h, 2p-2h and 4p-4h configurations relative to the lowest Nilsson determinant. Again one can expect that, beside the parameter describing the shape (η), the additional parameter ε (see Section 3.3.2) will be useful.

Work is in progress in Ljubljana [31] to calculate low lying states in (1d2s)-nuclei. The application to ^{16}O represents a microscopic counterpart to the Brown and Green model [32] and may or may not support that model.

3.3.4. Coupling of "quadrupole" and "pairing" vibrations

If one performs a constrained Hartree-Bogoljubov (CHB) calculation (as an approximation to PHB) with the pairing energy $\Delta_p = G \sum_\nu u_\nu v_\nu$ as constrained quantity [33] the curves of the binding energy for each rotational level, $E_J(\Delta_p)$ depending on Δ_p, are sometimes very shallow. For such J-states it is not senseful to look for a minimum in order to determine the intrinsic state-a superposition of Δ_p-dependent wave functions with the help of GCM is suggested to yield an improvement. Such kind of superposition has been used successfully for the description of pairing vibrational states in heavier nuclei [26] by using the parameter Δ which introduces a similar degree of freedom as Δ_p. Nevertheless there are nuclei like ^{24}Ne or ^{32}S whose spectra and transitions fit better into a vibrational scheme with large anharmonicities than into a rotational one. So we cannot expect to describe these spectra properly using only PHB or GCM with respect to Δ. We suggest a model of coupled "quadrupole - pairing vibrations" (β-Δ-coupling) incorporating both degrees of freedom in the framework of GCM. In this picture the total wavefunction Ψ_J of the system with total angular momentum J is written as

$$\Psi_J(x) = \int d\beta \int d\Delta \; f_J(\beta,\Delta)\Phi^{J,N}(x,\beta,\Delta)$$

The Hill-Wheeler equation has to be solved for each J-value sepa-

rately. $\Phi_J(x,\beta,\Delta)$ can be any appropriately chosen wavefunction depending on the quadrupole deformation and on a quantity Δ connected with the amount of pairing correlations. One could use wavefunctions obtained by a CHB calculation with quadrupole moment and pairing energy as constraints. In order to simplify the calculation we suggest to use N-projected BCS functions (obtained by solving the BCS equations) depending on Δ and the Nilsson single particle energies, which are functions of β. The two-parametric generator function $\Phi^{J,N}(x,\beta,\Delta)$ has the advantage that there is no trouble [27] in the limit $\Delta \to 0$ if one uses the BCS dependence of u and v on Δ and β.

In physical systems where the region of small Δ is important the one-parametric family $\Phi(x,\Delta)$ has the disadvantage that the amplitudes of 2p-2h and 4p-4h components are rather insensitive to changes in Δ, and therefore the $\Phi(x,\Delta)$ span a very small subspace. The two-parametric family $\Phi(x,\beta,\Delta)$, however, ensures more freedom for mixing 2p-2h, 4p-4h configurations with various amplitudes.

The calculation will be performed in three successive steps:

1. The calculation of the energy surface for a rather small set of mesh points $k = (\beta_k,\Delta_k)$ in the parameter space

$$E_k^J = \frac{\langle \Phi_J(x,\beta_k,\Delta_k)|H|\Phi_J(x,\beta_k,\Delta_k)\rangle}{\langle \Phi_J(x,\beta_k,\Delta_k)|\Phi_J(x,\beta_k,\Delta_k)\rangle} .$$

2. The calculation of the overlap matrix I_{ik}^J for a sufficient set of mesh points around the minimum of the energy surface E_k^J for all J values

$$I_{ik}^J = \langle \Phi_J(x,\beta_i,\Delta_i)|\Phi_J(x,\beta_k,\Delta_k)\rangle$$

   Diagonalization of I_{ik}^J will indicate the number of states we may expect in the sense we discussed in Sec.2.2.3.2.

3. The choice of the proper set of mesh points for each J-value in order to build up the energy matrix

$$H^J_{ik} = \langle \Phi_J(x,\beta_i,\Delta_i) | H | \Phi_J(x,\beta_k,\Delta_k) \rangle$$

and the solution of the Hill-Wheeler equations for each J separately

$$\sum_k (H^J_{ik} - E^J I^J_{ik}) f^J_k = 0 \quad \text{for all} \quad i.$$

The selection of a proper set of mesh points is a nontrivial problem common to all two-parametric GCM and is discussed in Section 2.3.1. If one wants to save computer time one can try to plot the energy surface and solve the Hill-Wheeler equation along the path of smallest ascent to obtain a description for low lying states.

The formalism for the calculation of the overlap matrix I^J_{ik} and the energy matrix H^J_{ik} can be obtained by generalizing the theory of ref. [18]:
One makes the Hartree-Bogoljubov transformation from the axially symmetric basic states c^+_a to the quasiparticles a^+_γ

$$a^+_\gamma = (\sum_a A_{a\gamma} c^+_a + B_{a\gamma} c_a)$$

By means of such quasiparticles one builds unprojected axially symmetric HFB states $|\Phi_i\rangle$ satisfying $a_\gamma|\Phi_i\rangle = 0$. With the rotational operator $\hat{R}(\phi) = \exp(i\phi \hat{J}_y)$ and the gauge transformation $\hat{S}(\theta) = \exp(i \frac{\hat{N}}{2} \theta)$ one writes the overlaps

$$n^{(i,k)}(\phi,\theta) = \langle \Phi_i | \hat{R}(\phi)\, \hat{S}(\theta) | \Phi_k \rangle$$

$$h^{(i,k)}(\phi,\theta) = \langle \Phi_i | \hat{H}\, \hat{R}(\phi)\, \hat{S}(\theta) | \Phi_k \rangle$$

which define the overlap matrix

$$I^J_{ik} = \frac{2J+1}{4\pi} \int_0^\pi d\phi \, \sin\phi \, d^J_{oo}(\phi) \int_0^{2\pi} d\theta \, \exp(-i \frac{N}{2} \theta) \, n^{(i,k)}(\phi,\theta)$$

and the energy matrix

$$H^J_{ik} = \frac{2J+1}{4\pi} \int_0^{\pi} d\phi \, \sin\phi \, d^J_{oo}(\phi) \int_0^{2\pi} d\theta \, \exp(-i \frac{N}{2} \theta) h^{(i,k)}(\phi,\theta)$$

The overlap functions can be expressed in terms of the HB transformation matrices A and B in the following form

$$n^{(i,k)}(\phi,\theta) = \left[\det \chi_{(i,k)}\right]^{1/2}$$

where

$$\chi_{(i,k)} = A^T_{(i)} \, R(\phi) \, A^*_{(k)} + B^T_{(i)} \, R(\phi) \, B^*_{(k)}$$

Similarly,

$$\frac{h^{(i,k)}(\phi,\theta)}{n^{(i,k)}(\phi,\theta)} = \sum_{ab} t_{ab} \, \rho^{(i,k)}_{ba} + \frac{1}{2} \sum_{abcd} V_{abcd} \, \rho^{(i,k)}_{ca} \, \rho^{(i,k)}_{db} +$$

$$+ \frac{1}{4} \sum_{abcd} V_{abcd} \, \kappa^{(i,k)}_{dc} \, \sigma^{(i,k)}_{ba}$$

where

$$\rho^{(i,k)}(\phi,\theta) = R(\phi) \, B^*_{(k)} \exp(i\theta) \, \chi^{-1}_{(i,k)} \, B^T_{(i)} \exp(i\theta)$$

$$\kappa^{(i,k)}(\phi,\theta) = \{R(\phi) \, B^*_{(k)} \exp(i\theta) \, \chi^{-1}_{(i,k)} \, A^T_{(i)}\}^T$$

$$\sigma^{(i,k)}(\phi,\theta) = R^*(\phi) \, A^*_{(k)} \, \chi^{-1}_{(i,k)} \, B^T_{(i)}$$

The β-Δ GC family will be used [34] to describe ^{24}Ne, since both quadrupole and pairing modes seem to be present. Also, the existing computer codes can be used without much modifications. The basis will be restricted to Nilsson states up to the 2s-1d shell. A realistic two body interaction will be used with the noncentral Hamada-Johnston force or the Yale force, taking the effective G-matrix elements of Barrett et al. [35] and of Shakin et al. [36].

Since all HB calculations of ^{24}Ne show pairing only between neutrons, pure Nilsson determinants for protons will be used what simplifies the N-projection.

The use of the β-Δ generator coordinate family will probably be most interesting for medium-heavy nuclei like Ni, Zn, Ge, Se isotopes. The single parametric families $\Phi(x,\Delta)$ or $\Phi(x,\beta)$ are not successful in these nuclei. Also, there is an unexplained surplus of low lying 0^+, 2^+, ... states, which might be due to coupling with the pairing vibrational degree of freedom.

3.4. Some difficulties in the association of intuitive picture of nuclear motion with the results of GCM calculations

Depending on the physical quantity P which has been used to select the subspace of the Hilbert space, it is customary to call the resulting solutions of the Hill-Wheeler equations P-vibrational states. Here one sees immediately the kind of ambiguity which this nomenclature introduces. It may happen in different calculations that the spaces spanned are very different. This is e.g. the case in Sec. 3.3.1. in which a quite different part of Hilbert space is used than in Secs. 3.2.2, and 3.2.4. Calling both solutions of the Hill-Wheeler equation P-vibrations is using the same name for different states.

On the other hand, it can happen that constraining two different physical quantities P and Q leads to essentially the same subspace; in this case the solutions of the Hill-Wheeler equation could equally well be called P or Q vibrations. A very clear example of this is provided by the Nilsson functions which are eigen functions of the Nilsson Hamiltonian with

$$V_{Nilsson} = \omega_o^2 r^2 + \beta r^2 Y_{20} + \xi \, \ell.s$$

Restricted to one major shell, the eigenfunctions of $V_{Nilsson}$

depend only on the ratio β/ξ. Keeping ξ constant and allowing β to vary generates exactly the same space of functions as when β is kept constant and ξ is allowed to vary. Carrying out a GC calculation using β as a generator coordinate will give exactly the same result as when ξ is used as a generator coordinate, so that the resulting states could equally well be called quadrupole vibrations or "spin-orbit-coupling" vibrations. Thus one has to be careful in sticking a classical picture and name onto the states obtained in a GCM calculation.

4. GENERATOR COORDINATE METHOD FOR NUCLEAR REACTIONS

For a long time, the resonating-group method [37] was the only practical framework for the calculation of nuclear scattering and reactions in terms of the nucleon-nucleon potential and with the Pauli principle properly taken into account. However, the extension of this method to the scattering of larger nuclei than the α-particle leads to very elaborate calculations.

The generator coordinate method offers a possibility to go to larger fragments. However, the applications of the generator coordinate method to the nuclear scattering is very recent and it is still at a pioneering stage.

In the following we shall review some results, work in progress and some new ideas about the use of GCM in nuclear scattering. Unlike in Ch.2 and Ch.3 we shall discuss the present status and the work in progress together - the application of the GCM to nuclear scattering is very recent and most publications are reports on the work in progress.

4.1. Description of scattering waves

To describe the relative motion of two nuclei one may start with a set of wave functions Φ depending on two types of parameters, the parameter r which is associated with the coordinate x describing the relative distance between two nuclei and parameters λ which generate changes in shape, orientation and size of scattering nuclei. The parameters λ correspond to generator coordinates in bound state problems. We shall concentrate first on the parameter r.

We shall restrict the choice of the generator function to such that can be written in the convenient form [37-39,5]

$$\Phi(x_i,r) = \Phi_{cm}\cdot\mathcal{A}\left[G(r,x).\ \Phi_A(x'_1,\ldots x'_A).\Phi_B(x'_{A+1}\ \ldots\ x'_{A+B})\right]. \quad (4.1)$$

Here $G(r,x)$ is some function peaked around $r = x$. The x_i' are the internal coordinates in the two nuclei A and B respectively. The wave functions Φ_A and Φ_B for the internal motion in the respective fragment nuclei are assumed to be antisymmetrised in themselves. The antisymmetriser $\mathcal{A}$ takes care of the exchange of nucleons between the two fragments. The centre of mass wave function Φ_{cm} does not introduce any spurious effects if it factors out exactly in the whole space of trial functions. It is included in (4.1) because Φ may then be as simple as a Slater determinant.

If the two nuclei are described by suitable shell model Slater determinants in two wells separated by a distance r and having the same value b of the oscillator parameter, the simple product determinant for the whole system has the form (4.1). In the α-cluster model of Brink, the Slater determinants may be written in the form (4.1) if all cluster size parameters b_i are equal. In this case $r = r_A - r_B$ where r_A is the centroid of the geometric figure defining the α-particle configuration A and r_B is defined analogously.

Both for the harmonic oscillator shell model and for the α-cluster model the function of relative motion G is

$$G(x,r) = (\sqrt{\pi}\beta)^{-3/2} e^{-(x-r)^2/2\beta^2} \qquad (4.2)$$

where $\beta^2 = b^2 \frac{m}{\mu}$. Here, b is the oscillator parameter and μ and m are the reduced mass of the system and the nucleon mass, respectively.

If we Fourier transform* the basis function defined by (4.1) (with G given by (4.2)) with respect to the parameter r we obtain a new set of functions labelled by a parameter q which is associated (at least outside the overlap region $|r| > R_A + R_B$) with the rela-

*The following notation will be used: all quantities in the momentum basis will be written with the same symbol as in the coordinate basis, but with a tilder.

tive momentum of the two nuclei

$$\tilde{\Phi}(x_i,q) = \Phi_{cm}\cdot\mathcal{A}\left[\left(\frac{\sqrt{\pi}}{\beta}\right)^{-3/2} e^{-(\beta^2 q^2)/2}\; e^{iq\cdot x}\; \Phi_A\; \Phi_B\right] \qquad (4.3)$$

If one renormalises these functions by a factor $(2\sqrt{\pi}\beta)^{-3/2}\cdot e^{\beta^2 q^2}$ one obtains - except for the centre of mass factor - just the resonating group wave functions [38] with normalised plane waves as the relative motion functions.

Wong [41] has suggested a more general way of constructing resonating group wave functions on the basis of Slater determinants. For each nucleus Wong uses wave functions of Peierls-Thouless type, e.g.:

$$\tilde{\Phi}_A(x_i;q_A;p_A) = e^{iq_A\cdot x_A}\cdot e^{-ip_A\cdot x_A}\cdot\int e^{ip_A\cdot\alpha}\cdot\Phi_A^D(x_i-\alpha)\,d^3\alpha \qquad (4.4)$$

where Φ_A^D is a Slater determinant for the nucleons in nucleus A and x_A is its center of mass. The first factor $e^{iq_A x_A}$ ensures that the centre of mass wave function for this nucleus is a plane wave with momentum q_A. The second factor cancels with the term $e^{+ip_A x_A}$ resulting from the momentum projection from the Slater determinant Φ_A^D. Thus the last two factors just make up an intrinsic state Φ_A which only depends on the internal coordinates $x_i' = x_i - x_A$.

The parameter p_A, which may label some internal degree of freedom in the nucleus A, is redundant if Φ_A^D already factors into centre of mass and intrinsic wave functions. One may rewrite (4.4)

$$\tilde{\Phi}_A(x_i;q_A;p_A) = \int d^3\alpha\cdot e^{ip_A\cdot\alpha}\cdot\Phi_A^{D'}(q_A-p_A,x_i-\alpha) \qquad (4.4')$$

to see that Φ_A is just an integral over the determinantal wave functions

$$\tilde{\Phi}_A^{D'}(q_A-p_A,x_i-\alpha) = e^{i(q_A-p_A)\cdot x_A}\cdot\Phi_A^D(x_i-\alpha)\ .$$

The basis states of the system of two nuclei are now the anti-symmetrised products of two such wave functions Φ_A, Φ_B.

$$\tilde{\Phi}(x_\ell;q;p_A,p_B) = \mathcal{A}\left[\tilde{\Phi}_A(x_i;q_A,p_A).\tilde{\Phi}_B(x_J;q_B,p_B)\right]$$

$$= e^{i(q_A+q_B)x_{cm}}\,\mathcal{A}\left[e^{iq.x}.\tilde{\phi}_A(x'_i,p_A).\tilde{\phi}_B(x'_J,p_B)\right] \qquad (4.5)$$

$$= \int d^3\alpha \int d^3\beta\; e^{ip_A.\alpha}.e^{ip_B.\beta}\,\mathcal{A}\left[\tilde{\phi}_A^{D'}(q_A-p_A,x_i-\alpha).\tilde{\phi}_B^{D'}(q_B-p_B,x_j-\beta)\right].$$

The second line of (4.5) shows that the relative motion wave function is a plane wave of momentum $q = q_A - q_B$. The third line of (4.5) illustrates the nature of the basis state, being an integral over Slater determinants

$$\Phi_D(x_1,\ldots x_A,x_{A+1},\ldots x_{A+B}) = \mathcal{A}\left[\Phi_A^{D'}.\Phi_B^{D'}\right] . \qquad (4.6)$$

Generalizations. In both coordinate and momentum representations, the shell model functions Φ (eq. 4.1 and 4.2) or Φ_D (eq. 4.6) are Slater determinants (or superpositions of Slater determinants) and the calculation of the Hill-Wheeler kernels is possible with standard second quantization techniques. So far, the factorization property, eq. (4.1), has been assumed to hold for all values of r, which physically corresponds to the sudden approximation. It may be physically more interesting to relax this condition in the interaction region. Comming back to eq. (4.1), a generalization consists in taking for $\Phi(x_\ell,r)$ when $|r| < R_o$, the result of a constrained Hartree Fock calculation [21] (slow adiabatic limit) or of a two center shell model calculation or of any other suitable approximation. Analogous generalization of eq. (4.5) is

$$\tilde{\Phi}(x_i,q,p_A,p_B) = \int d^3\alpha \int d^3\beta \; e^{ip_A\alpha} \; e^{ip_B\beta}$$

$$\mathcal{A}\left[e^{i(q-p_A)x_A} \; e^{-i(q+p_B)x_B} \; \Phi^D_{A+B,\alpha-\beta}(x_i-\alpha,x_j-\beta)\right] \qquad (4.7)$$

where the additional index $\alpha-\beta$ in the determinant $\Phi^D_{A+B,\alpha-\beta}$ indicates the dependence of the compound nucleus wave function on $\alpha-\beta$ in the interaction region $|\alpha-\beta| < R_o$.

Tabakin [42] generalized the function (4.1) by introducing an additional generator coordinate λ which describes the changes of nuclear shape, size and orientation during the collision,

$$\Phi^\lambda(x_i,r) = \Phi_{CM} \cdot \mathcal{A}\left[G(r,x)\Phi^{\lambda_A}_A(x'_1,\ldots x'_A)\Phi^{\lambda_B}_A(x'_{A+1},\ldots,x'_{A+B})\right] \quad (4.8)$$

The corresponding trial function is

$$\Psi(x_i) \equiv \int\int d\lambda \; d^3r \; \Phi^\lambda(x_i,r) \; .$$

The generator coordinate $\lambda \equiv(\lambda_A,\lambda_B)$ generates certain inelastic channels in the asymptotic region. So the coupling between such channel and the elastic channel is included in this type of generator function.

In the following (Sec.4.2.1) we shall use also an alternative generalization of the generator function (4.1) to several channels. Then we have n sets of generator functions

$$\Phi_c(x_i,r) = \Phi_{CM} \; \mathcal{A}\left[G_c(r,x)\Phi_{Ac}(x'_1,\ldots)\Phi_{Bc}(x'_{A+1},\ldots)\right] \qquad (4.9)$$

The product $\Phi_{Ac}\Phi_{Bc}$ represents different intrinsic states of the separated nuclei and will be assumed to be diagonalized with respect to the Hamiltonian H_A+H_B of the internal motion of the scattered nuclei,

$$\langle\Phi_{Ac'}\Phi_{Bc'}|(H_A + H_B)|\Phi_{Ac}\Phi_{Bc}\rangle = E_c \; \delta_{cc'} \qquad (4.10)$$

The trial function is then

$$\Psi(x_i) = \sum_{c=1}^{n} \int d^3r f_c(r)\Phi_c(x_i,r) \qquad (4.11)$$

4.2. Solution of Hill-Wheeler equation for scattering boundary conditions

In this chapter we review methods for solving the Hill-Wheeler equation when the generator functions are either $\Phi_c(x_i,r)$, eq. (4.9), with a relative motion function

$$G_c(x,r) = (\sqrt{\pi}\ \beta_c)^{-3/2}\ e^{-(x-r)^2/2\beta_c^2} \qquad (4.12)$$

or $\phi^\lambda(x_i,r)$, with a relative motion function

$$G^\lambda(x,r) = (\sqrt{\pi}\ \beta_\lambda)^{-3/2}\ e^{-(x-r)^2/2\beta_\lambda{}^2} \qquad (4.13)$$

In the first case we have the system of n coupled integral equations of one variable r'

$$\sum_{c'} \int d^3r' \left[H_{cc'}(r,r') - EI_{cc'}(r,r')\right] f_{c'}(r') = 0\ , \qquad (4.14)$$

where

$$\begin{aligned} I_{cc'}(r,r') &= \langle \Phi_c(x_i,r) | \Phi_{c'}(x_i,r') \rangle \\ H_{cc'}(r,r') &= \langle \Phi_c(x_i,r) | H | \Phi_{c'}(x_i,r') \rangle \end{aligned} \qquad (4.15)$$

In the second case we have the integral equation of two variables λ and r,

$$\iint d\lambda'\ d^3r' \left[H(r,\lambda;r',\lambda') - EI(r,\lambda;r',\lambda')\right] f(\lambda',r') = 0 \qquad (4.16)$$

with

$$I(r,\lambda;r',\lambda') = \langle \Phi^{\lambda}(x_i,r) | \Phi^{\lambda'}(x_i,r') \rangle$$

$$H(r,\lambda;r',\lambda') = \langle \Phi^{\lambda}(x_i,r) | H | \Phi^{\lambda'}(x_i,r') \rangle \qquad (4.17)$$

4.2.1. Solution in momentum representation

Let us first write results for one channel (n=1). Then equation (4.14) may be transformed into an equivalent Schrödinger equation by the method first introduced by Giraud and Zaikine [38]. To do this one introduces the operator Γ which is defined by

$$\Gamma f(r) \equiv (\sqrt{\pi}\,\beta)^{-3/2} \int e^{-((x-r)^2/2\beta^2)} f(r) d^3r \equiv g(x) \qquad (4.18)$$

As we have assumed the Gaussian form (4.2) for $G(x,r)$ the function $g(x)$ is essentially $g(x) = \int G(x,r) f(r) d^3r$, i.e. $g(x)$ is asymptotically the relative part of the scattering wave function. The operators H and I may now be written as

$$H = -\Gamma \frac{\hbar^2}{2\mu} \Delta_r \Gamma + v \qquad (4.19a)$$

$$I = \Gamma^2 + n \qquad (4.19b)$$

where n and v are short ranged non-local operators with square integrable kernels $n(r,r')$ and $v(r,r')$. The operator n originates from the antisymmetrisation which causes $I(r,r')$ to deviate from its asymptotic form $e^{-(r-r')^2/4\beta^2}$. The operator v originates from the potential which is assumed to be short ranged, as well as from corrections to the kinetic energy of relative motion due to antisymmetrisation. Asymptotically this kinetic energy contributes a term

$$\left(3 - \frac{(r-r')^2}{2\beta^2}\right) \cdot \frac{\hbar^2}{4\mu\beta^2} \cdot e^{-(r-r')^2/4\beta^2}$$ to the kernel $H(r,r')$ and it is this term which gives $-\Gamma \frac{\hbar^2}{2\mu} \Delta_r \Gamma$ in (4.19a).

Additional contributions to $n(r,r')$ and $v(r,r')$ may come from deviations of the basis states $\Phi(r)$ from the form (4.1) in the interaction region. These deviations will not add any complications if the Hill-Wheeler kernels are to be calculated numerically, provided that these effects are of short range so that the form (4.1) is still valid asymptotically.

The equivalent Schrödinger equation for $g = \Gamma f$ now reads

$$\frac{\hbar^2}{2\mu} \Delta_r g + \Gamma^{-1} v \Gamma^{-1} g - E\Gamma^{-1} n \Gamma^{-1} g = Eg \ . \tag{4.20}$$

In momentum space the operator Γ^{-1} has the simple form:

$$\Gamma^{-1}\tilde{g}(q) = (2\sqrt{\pi}\ \beta)^{-3/2}\ e^{\beta^2 q^2/2}.\tilde{g}(q) \tag{4.21}$$

so that the kernels of the operators

$$w = \Gamma^{-1} v \Gamma^{-1} \quad \text{and} \quad \eta = \Gamma^{-1} n \Gamma^{-1} \tag{4.22}$$

can be calculated in momentum space by Fourier transforming $v(r,r')$ and $n(r,r')$ and multiplying by $(2\sqrt{\pi}\ \beta)^{-3}.e^{\beta^2 q^2/2}.e^{\beta^2 q'^2/2}$.

Although the operator Γ^{-1} is singular, the operators w and η have been shown to be regular in all practical calculations done so far.

In momentum space, the equivalent Schrödinger equation has the explicit form:

$$\begin{aligned} &\frac{\hbar^2}{2\mu} \cdot q^2.\tilde{g}(q) + \int d^3q'\tilde{w}(q,q').\tilde{g}(q')d^3q' \\ &- E(\tilde{g}(q) + \int d^3q'\tilde{\eta}(q,q')\tilde{g}(q')) = 0 \end{aligned} \tag{4.23}$$

Generalization to several channels is staightforward if we assume that the relative motion wave functions $G_c(x,r)$ are all

Gaussians as in (4.2), with channel dependent widths β_c. Then the expressions for the kernels (4.15) are:

$$I_{cc'}(r,r') = \delta_{cc'} e^{-\frac{(r-r')^2}{4\beta_c^2}} + n_{cc'}(r,r')$$

$$H_{cc'}(r,r') = \delta_{cc'} \left[\frac{\hbar^2}{4\mu\beta_c^2}\left(3 - \frac{(r-r')^2}{2\beta_c^2}\right) + E_c\right] e^{-\frac{(r-r')^2}{4\beta_c^2}} + v_{cc'}(r,r') \qquad (4.24)$$

where $n_{cc'}(r,r')$ and $v_{cc'}(r,r')$ are short ranged and square integrable.

The generalised operator Γ is defined by:

$$\Gamma f_c(r) \equiv (\sqrt{\pi}\,\beta_c)^{-3/2} \int e^{-\frac{(r-r')^2}{2\beta_c^2}} f_c(r')d^3r' \equiv g_c(r') \qquad (4.25)$$

or, in momentum space:

$$\Gamma \tilde{f}_c(q) \equiv (2\sqrt{\pi}\,\beta_c)^{3/2} e^{-\frac{\beta_c^2 q^2}{2}} \tilde{f}_c(q) \equiv \tilde{g}_c(q) \qquad (4.25')$$

The coupled channel Schrödinger equation in momentum space now has the form:

$$\frac{\hbar^2}{2\mu} q^2 \tilde{g}_c(q) + \sum_{c'} \int d^3q' \tilde{w}_{cc'}(q,q')\tilde{g}_{c'}(q') - (E-E_c)\tilde{g}_c(q) - E.\sum_{c'} \int d^3q' .\tilde{\eta}_{cc'}(q,q')\tilde{g}_{c'}(q') = 0 \qquad (4.26)$$

with

$$\tilde{\eta}_{cc'}(q,q') = (2\sqrt{\pi\beta_c\beta_{c'}})^{-3} e^{+\frac{\beta_c^2 q^2}{2}} \tilde{n}_{cc'}(q,q') e^{+\frac{\beta_{c'}^2 q'^2}{2}}$$

and

$$\tilde{w}_{cc'}(q,q') = (2\sqrt{\pi\beta_c\beta_{c'}})^{-3}\, e^{+\frac{\beta_c^2 q^2}{2}}\, \tilde{v}_{cc'}(q,q')\, e^{+\frac{\beta_{c'}^2 q'^2}{2}}, \quad (4.27)$$

The internal energies E_c in each channel are defined by (4.10).

4.2.2. Solution in coordinate representation

The solution of the Hill-Wheeler equation for scattering in the coordinate representation is quite different from that of the momentum representation. The reason is, that the generator functions $\Phi(x_\ell,r)$, eq. (4.1), are not orthogonal for different r, while the functions $\tilde{\Phi}(x_\ell,q)$, eqs. (4.3), (4.5) and (4.7), are almost orthogonal in the sense that $\langle\tilde{\Phi}(x_\ell,q)|\tilde{\Phi}(x_\ell,q')\rangle = \delta(q-q')+\tilde{\eta}(q,q')$, where $\tilde{\eta}(q,q')$ is bounded and its Fourier transform $\eta(r,r')$ is short range. This operator η is square integrable.

The problem is thus twofold (i) how to reduce an equation $(H - EI)f = 0$ to the diagonalization of a matrix, (ii) how to impose boundary conditions to the unknown f or to any related unknown of the problem, and how to make use of these boundary conditions to obtain phase shifts?

As regards the boundary conditions near the origin, which are related to Pauli principle, a complete solution is given by two authors [38,45]. It consists in a proper renormalization of $\phi(x_\ell,\alpha)$ when $\alpha \to 0$ or in the identification of "forbidden" waves f^c or g^c, for which the trial function Ψ cancels out identically, and which therefore arise as spurious "zero energy bound states". (These states may shift the value of the phase shift at zero energy by a multiple of π according to Levinson's theorem).

A first "direct" treatment [40], which is prepared for the solution of the Hill-Wheeler equation in coordinate space, takes f as the basic unknown. It may be described as follows:

(i) put the scattering system in a box of radius R and, in that box, discretize the Hill-Wheeler equation as

$$\sum_j (H_{ij} - EI_{ij}) f_j = - \int_R \left[H(r,r') - EI(r,r')\right] f(r') dr'$$

(ii) the right hand side may be taken as zero or tabulated according to which ansatz is made concerning the behaviour of f outside of the box. A boundary constraint has to be used. One may take advantage of eq. (4.21) or (4.25) to perform numerical integration of Γf_j and generate numerically the discretized values g_j of the scattering wave function g; then a matching of g_j to the usual asymptotic scattering (Coulomb) waves gives the phase shift. De Takacsy, however, used the matching for f.

(iii) The above matrix equation (i) can be solved by standard methods (Schmidt orthonormalization procedure) for the unknown f_j.

A second method consists in looking for an operator C for a transform of the equation of the unknown so that $(C^+)^{-1} I C^{-1}$ is the unit operator except possibly for a minor correction Ω. The new unknown is the function C f and the transform equation reads

$$\left[(C^{-1})^+ H C^{-1} - E(1+\Omega)\right] Cf = 0 \ ,$$

(see eq. (4.20)). In practical cases the simplest choice is to take $C = \Gamma$, where Γ was defined by eq. (4.18). This choice has the great advantage that the new known is the physical scattering wave $g = \Gamma f$, the boundary conditions of which are well unknown. Also, it is easy to see that in the asymptotic region, $I \to \Gamma^+\Gamma$, so that indeed $\Omega \equiv (\Gamma^+)^{-1} I \Gamma^{-1} - 1$ may be considered as a short range, "minor" correction. Thus $(\Gamma^+)^{-1} H \Gamma^{-1} = E\Omega$ may be considered as the optical Hamiltonian which governs the scattering wave g. There is a difficulty, of course, in this method, because the inversion of Γ in coordinate representation is in general not a straightforward problem. If this difficulty can be resolved, it is reasonable to claim that this method of "Γ transform" is the most interesting

physically. If, however, an inversion of Γ (or more generally C) is not possible exactly, one must turn to the first method described above or to other methods such as listed below.

A third method [5] consists in looking for an operator D such that ID^{-1} or $D^{-1}I$ (rather than $(C^+)^{-1}IC^{-1}$) is a unit operator except for a possible correction Ω'. The transformed equation thus reads $(HD^{-1}-E\Omega')\,(Df) = E(Df)$. The most natural choice is of course D=I, leading to $\Omega' = 0$. It is clear, however, that the inversion of D (or I) is usually as much a difficult problem as the inversion of C (or Γ) which was discussed above. Also in general HD^{-1} is not hermitian and the physical meaning of the new unknown Df has to be defined as, for instance, the generator coordinate amplitude with respect to the biorthogonal basis of the basis $\{\Phi(x_\ell,r)\}$ (if such a biorthogonal basis exists!). It may be difficult to interpret HD^{-1} as an optical Hamiltonian, and it may be concluded that this last method is of interest only if HD^{-1} is very simple to obtain.

A fourth method consists in transforming the integral kernels H and I into series of differential operators. For instance

$$I(r,r') = \sum_{p=o}^{\infty} \frac{1}{p!} I_p(r)\left(\frac{d}{dr}\right)^p$$

where $I_p(r)$ are moments $\int dr' I(r,r')(r-r')^p$. One then truncates the series after a given order (usually after second order terms p=2) and the Hill-Wheeler equation is thus approximated by a second order differential equation. It is clear that great care must be exercised in order to check the hermiticity and convergence in such procedures.

As the last, let us note a method which is close to the Kohn variational method [44]. This method consists in splitting Ψ into an inner part and an asymptotic part

$$\Psi_{inner} = \int_o^{R_o} dr\, f(r)\Phi(x_\ell,r)$$

$$\Psi_{asymp} = \int_{R_o}^{\infty} dr\ f(r)\Phi(x_\ell, r) \quad .$$

In order to identify channels, the representation of Ψ_{asymp} in a basis like (4.1) is necessary. On the other hand, Ψ_{inner} may be expanded in many ways: in a GC basis $\Phi(x_\ell, r)$ or a discrete orthonormalized shell model basis $\Phi_i(x_\ell)$. A prediagonalization is possible, so that $\langle\Phi_i|H|\Phi_j\rangle = E_i\ \delta_{ij}$. With such a mixed representation, Ψ reads

$$\Psi(x_\ell) = \sum_i f_i\Phi_i(x_\ell) + \int_{R_o}^{\infty} dr\ f(r)\Phi(x_\ell, r)$$

The resulting modified Hill-Wheeler equation is

$$\int_{R_o}^{\infty} dr' \Big[\langle\Phi(x_\ell, r)|H-E|\Phi(x_\ell, r')\rangle +$$

$$+ \langle\Phi(x_\ell, r)|(H-E)\sum_i \frac{|\Phi_i(x_\ell)\rangle\langle\Phi_i(x_\ell)|}{E_i - E \pm i\varepsilon}(H-E)|\Phi(x_\ell, r')\rangle\Big] f(r') = 0$$

$$f_i^{\pm} = -\frac{1}{E-E_i\pm i\varepsilon}\int_{R_o}^{\infty} dr\ f(r)\langle\Phi_i(x_\ell)|H-E|\Phi(x_\ell, r)\rangle$$

This method may be suitable for a study of resonances.

Not enough experience in numerical and analytical calculations is as yet available to decide which of the various methods is to be prefered. Clearly the Γ-transform method is easiest to interpret but it is preferable only when the calculation of $\Gamma^{-1}I\Gamma^{-1}$ and $\Gamma^{-1}H\Gamma^{-1}$ is not too difficult. In most cases, the "direct" method (solving for f) may be simpler if no optical potentials are looked for.

4.2.3. Decomposition into spherical waves for the scattering of spinless fragments

For the actual solution of equation (4.14) or equation (4.23) it is practical to expand the kernels $H_{cc'}(r,r')$ and $I_{cc'}(r,r')$ in spherical harmonics:

$$H_{cc'}(r,r') = \sum_{L,M} Y_{LM}(\theta,\phi) H^{L}_{cc'}(r,r') Y^{*}_{LM}(\theta',\phi')$$

$$I_{cc'}(r,r') = \sum_{L,M} Y_{LM}(\theta,\phi) I^{L}_{cc'}(r,r') Y^{*}_{LM}(\theta',\phi') \quad . \tag{4.28}$$

Such an expansion ($\sum_{L,M}$ rather than $\sum_{L,L',M,M'}$) is possible only if the integral operators H and I commute with rotations $R_r(\Omega)$ of the parameter r. This is not trivially fulfilled since r is associated with the angular momentum L of the relative motion of the two nuclei and L is only asymptotically a good quantum number.

Let us assume that the trial states $\Phi_c(x_\ell,r)$ are constructed such, that a rotation $R_r(\Omega)$ of the parameter r through some Euler angles Ω is equivalent to a rotation $R_\Phi(\Omega)$ of the whole wave function Φ_c (except the centre of mass part) through the same angles,

$$R_r(\Omega) = R_\Phi(\Omega) \tag{4.29}$$

Condition (4.29) is fulfilled for the generator function of the form

$$\Phi_c(x_\ell,r) = \Phi_{cm}\, \mathcal{A}\left[G((r-x)^2)\Phi_{Ac}(x'_i)\Phi_{Bc}(x'_j)\right] \tag{4.30}$$

if the internal wave functions Φ_{Ac} and Φ_{Bc} of the two nuclei are spin 0 states (as for example in the $\alpha+\alpha$ system when the α-particles are in harmonic oscillator ground states). If (4.29) is fulfilled for all channels c, then it follows from the rotational invariance

of the operators H and I in Hilbert space, that the integral operators H and I, eq. (4.15) commute with rotations of r, and the expansions (4.28) are justified.

The Hill-Wheeler equations (4.14) can then be solved with an ansatz

$$f_c(r) = f_c^L(r).Y_{LM}(\theta,\phi) \ , \tag{4.31}$$

leaving us with equations for the radial function $f_c^L(r)$:

$$\sum_{c'=1}^{n} \int_0^\infty r'^2 dr' \left[H_{cc'}^L(r,r') - EI_{cc'}^L(r,r')\right] f_{c'}^L(r') = 0 \tag{4.32}$$

(for all c and all r values)

The $H_{cc'}^L$ and $I_{cc'}^L$ of equation (4.28) are obtained by multiplying $H_{cc'}(r,r')$ resp. $I_{cc'}(r,r')$ on the left and right by spherical harmonics and integrating over all angles. Using the expressions (4.28) for $H_{cc'}(r,r')$ and $I_{cc'}(r,r')$ one sees that the L-dependent kernels $H_{cc'}^L(r,r')$ and $I_{cc'}^L(r,r')$ are just the matrix elements of the operators H and 1 between basic states with projected angular momentum:

$$\begin{aligned} H_{cc'}^L(r,r') &= \langle \Phi_c(re_z) | H P_{oo}^L | \Phi_{c'}(r'e_z') \rangle \\ I_{cc'}^L(r,r') &= \langle \Phi_c(re_z) | P_{oo}^L | \Phi_{c'}(r'e_z) \rangle \end{aligned} \tag{4.33}$$

where e_z is a unit vector in direction of some fixed z-axis.

Like in (4.24) we separate the kernels $H_{cc'}^L(r,r')$ and $I_{cc'}^L(r,r')$ into short and a long range terms

$$I_{cc'}^L = (2L+1)\, i^{-L}\, e^{-\frac{r^2+r'^2}{4\beta_c^2}}\, j_L\left(i\,\frac{rr'}{2\beta_c^2}\right) \delta_{cc'} + n_{cc'}^L(r,r')$$

$$H^L_{cc'} = (2L+1)\, i^{-L}\, e^{-\frac{r^2+r'^2}{4\beta_c^2}} \{E_c j_L(i\frac{rr'}{2\beta_c^2}) + \frac{\hbar^2}{4\mu\beta_c^2}(3-\frac{r^2+r'^2}{2\beta_c^2}) j_L(i\frac{rr'}{2\beta_c^2})$$

$$+ \frac{\hbar^2}{4\mu\beta_c^2}\, i.\frac{rr'}{\beta_c^2}\, j'_L(i\frac{rr'}{2\beta_c^2})\}\delta_{cc'} + v^L_{cc'}(r,r') \qquad (4.34)$$

Here $n^L_{cc'}(r,r')$ and $v^L_{cc'}(r,r')$ are obtained from $n_{cc'}(r,r')$ and $v_{cc'}(r,r')$ by an expansion as in (4.28). In practice $n^L_{cc'}(r,r')$ and $v^L_{cc'}(r,r')$ will be obtained by merely subtracting the long range terms appearing in (4.34) from the kernels $H^L_{cc'}(r,r')$ and $I^L_{cc'}(r,r')$ which can be calculated numerically.

In momentum space an expansion of the form (4.28) can also be made and the kernels $\tilde{H}^L_{cc'}(q,q')$, $\tilde{I}^L_{cc'}(q,q')$, $\tilde{v}^L_{cc'}(q,q')$ and $\tilde{n}^L_{cc'}(q,q')$ can be obtained from the corresponding kernels in coordinate space by transformations of the following type:

$$\tilde{n}^L_{cc'}(q,q') = \frac{2}{\pi}\int_0^\infty r^2dr \int_0^\infty r'^2dr' j_L(qr) j_L(q'r') n^L_{cc'}(r,r')$$

$$\tilde{v}^L_{cc'}(q,q') = \frac{2}{\pi}\int_0^\infty r^2dr \int_0^\infty r'^2dr' j_L(q,r) j_L(q'r') v^L_{cc'}(r,r') \qquad (4.35)$$

The long range parts of the kernels (4.34) can be transformed analytically to the momentum space:

$$\tilde{I}^L_{cc'}(q,q') = (2\sqrt{\pi}\,\beta_c)^3\, e^{-\frac{\beta_c^2 q^2}{2}} \frac{\delta(q-q')}{q.q'} e^{-\frac{\beta_c^2 q'^2}{2}} \delta_{cc'} + \tilde{n}^L_{cc'}(q,q')$$

$$\tilde{H}^L_{cc'}(q,q') = (2\sqrt{\pi}\,\beta_c)^3\, e^{-\frac{\beta_c^2 q^2}{2}} \cdot \frac{\hbar^2}{2\mu}\delta(q-q') e^{-\frac{\beta_c^2 q'^2}{2}} \cdot \delta_{cc'} + \tilde{v}^L_{cc'}(q,q') \qquad (4.36)$$

The coupled channel equations for the radial parts $\tilde{g}^L_c(q)$ of the functions $\tilde{g}_c(q) = \Gamma\tilde{f}_c(q)$ are now

$$\frac{\hbar^2}{2\mu} q^2 \tilde{g}_c^L(q) + \sum_{c'=1}^{n} \int_0^\infty q'^2 dq' \tilde{w}_{cc'}^L(q,q') \tilde{g}_{c'}^L(q')$$

$$- (E-E_c) \tilde{g}_c^L(q) - E \sum_{c'=1}^{n} \int_0^\infty q'^2 dq' \tilde{\eta}_{cc'}^L(q,q') \tilde{g}_{c'}^L(q') = 0 \,, \tag{4.37}$$

where

$$\tilde{\eta}_{cc'}^L(q,q') = (2\sqrt{\pi\beta_c\beta_{c'}})^{-3} e^{+\frac{\beta_c^2 q^2}{2}} \tilde{n}_{cc'}^L(q,q') e^{+\frac{\beta_{c'}^2 q'^2}{2}}$$

$$\tilde{w}_{cc'}^L(q,q') = (2\sqrt{\pi\beta_c\beta_{c'}})^{-3} e^{+\frac{\beta_c^2 q^2}{2}} \tilde{v}_{cc'}^L(q,q') e^{+\frac{\beta_{c'}^2 q'^2}{2}} \tag{4.38}$$

4.2.4. Remarks concerning the calculation of the phase shift for noncharged particles

The relation between the potential $\tilde{w}(q,q')$ eq. (4.27), and the phase shift is known from literature [46]. One defines the matrix $\tilde{K}$ as:

$$\tilde{K}(q,k) = \tilde{w}(q,k) + \int_0^\infty \tilde{w}(q,k) \frac{1}{q'^2-k^2} \tilde{K}(q',k) q'^2 dq' \,. \tag{4.39}$$

The phase shift $\tilde{\eta}(k)$ is then expressed in terms of on-shell matrix element of $\tilde{K}$,

$$\tilde{K}(k,k) = - \frac{2k}{\pi} \operatorname{tg} \tilde{\eta}(k) \,, \tag{4.40}$$

where k is the momentum corresponding to the given energy $E = (\hbar^2/2\mu)k^2$. The eq. (4.39) can be solved numerically [39].

In coordinate representation De Takacsy [40] showed that the phase shifts of the functions $f(r)$ and $g(x)$ are the same. This follows immediately from the eq. (4.18) which is valid in asymptotic region.

4.2.5. Coulomb scattering

So far, in most applications of GCM in nuclear scattering the Coulomb potential was not included. In the following we would like (i) to note that there exists a recipe how to include the contribution of the Coulomb force if the calculation is performed in momentum representation; (ii) we shall present the theorem that the functions $g(x)$ and $f(r)$ related by eq. (4.18) have the same phase shifts (at least up to corrections of the order $1/r^2$). This is important in calculations in coordinate representation.

(i) The calculation of phase shifts in momentum representation does not allow long range potentials ($\sim 1/r$). So, sometimes the following recipe is used: calculate the phase shift by eq.(4.40) for the nuclear and the truncated Coulomb potential (I) shown in Fig. 4.1. Then subtract from the obtained phase shift the value $\left[L(L+1) + (Z_1 Z_2 e^2/\hbar v)^2\right]/2kR_o$ corresponding to the part II of the Coulomb potential.

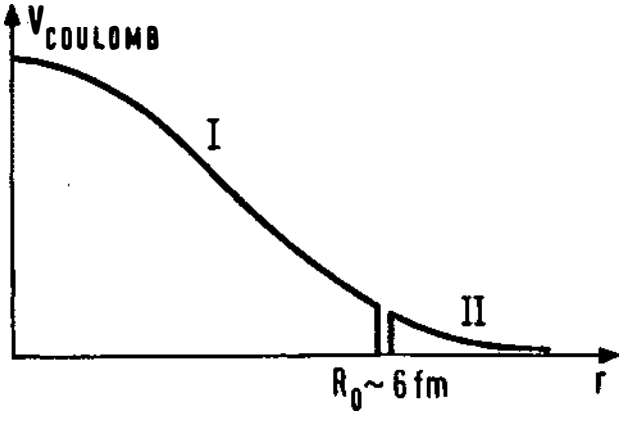

Fig. 4.1 The stape of the potential used in the calculation of the phase shifts due to the Coulomb force.

(ii) If the calculation is performed in the coordinate representation, it is usually more convenient to calculate $f(r)$, while the physical phase shift is given by $g(x)$. Therefore the following theorem may be useful. If for large x $g_L(x)$ behaves like a Coulomb wave then $f_L(r)$ has the same behaviour apart from a correction factor

$$\{1 - \frac{b^2 Z_1 Z_2 e^2 \mu}{\hbar^2} \cdot \frac{1}{r} + O(\frac{1}{r^2})\}, \quad r \to \infty \ .$$

As the term $O(\frac{1}{r})$ is real, the phase shifts may be affected at most by terms $O(1/r^2)$.

This asymptotic relation between f and g can be easily derived by assuming that the generating function $\Phi(x,r)$ has the asymptotic form (4.1), (4.2)

$$\Phi(x,r) \sim \exp\{-(x-r)^2/2b^2\}\ \Phi_{int} \ .$$

The antisymmetrization operator $\mathcal{A}$ in (4.1) was omitted in the limit $r \to \infty$. Then the asymptotic form of

$$\Psi(x_i) = \int \Phi(x_i,r) f(r) d^3r$$

for $x \to \infty$ is

$$\Psi(x_i) \sim \Phi_{int} \int \exp\{-(x-r)/2b^2\} f(r) d^3r = \Phi_{int}\ g(x) \ ,$$

where as in eq. (4.18).

$$g(x) = \int \exp\{-(x-r)^2/2b^2\}\ f(r) d^3r \ . \qquad (4.18')$$

As Φ_{int} does not depend on x, the asymptotic relative motion and the phase shifts are given just by the function $g(x)$. In our case $g(x)$ in the asymptotic region are Coulomb waves:

$$g_L^{\pm}(x) = \frac{1}{x}\left[1 + \frac{A_L}{x} + O(\frac{1}{x^2})\right] \exp\left[\pm i(kx - \gamma \ln 2kx - L\pi/2 + \delta_L)\right]$$

where $A_L = (i\gamma - L)(i\gamma + L + 1)/2i$ and, with obvious notation,

$$\gamma = \frac{Z_1 Z_2 e^2 \mu}{\hbar^2 k}, \qquad \mu = \frac{m_1 m_2}{m_1 + m_2} .$$

To perform the proof we make the ansatz for $f_L(\alpha)$

$$f_L^{\pm}(r) = \text{const.}\ \frac{1}{r}\left[1 + (A_L + a_L)/r + O(1/r^2)\right]$$

$$\cdot \exp\left[\pm i(kr - \gamma \ln 2kr - L\pi/2 + \delta_L)\right]$$

and check whether it reproduces $g_L(x)$ from (4.18') up to terms of $O(1/x^2)$,

$$g_L^{\pm}(x) = \text{const.}\left[1 + A_L/x + O(1/x^2)\right] \int_0^{\infty} r^2 dr\ j_L(i\,xr/b^2) \cdot$$

$$\cdot \exp\left[-(x^2+r^2)/2b^2\right] f_L(r)$$

For large x we have $j_L(ixr/b^2) \sim i^{-L} \frac{b^2}{2xr} \exp(xr/b^2)(1 + C_L b^2/xr + \ldots)$ where C_L are the corresponding expansion coefficients. Then for large x (and $r = x+t$) we have

$$g_L^{\pm}(x) \sim i^{-L}(b^2/2x) \int_0^{\infty} dt\ \exp(-t^2/2b^2) \cdot$$

$$\exp\left[\pm k(x+t) - \gamma \ln 2k(x+t) + \delta_L\right] \cdot$$

$$\cdot\left[1 + \frac{C_L b^2}{x(x+t)} + \ldots\right]\left[1 + \frac{A_L + a_L}{x+t} + O\left(\frac{1}{(x+t)^2}\right)\right]$$

$$= i^{-L} \frac{b^2}{2x} \exp(\mp \gamma \ln 2) \exp\left[\pm i(kx - \gamma \ln 2kx + \delta_L)\right] \cdot$$

$$\int_{-x}^{\infty} dt\ \exp(-t^2/2b^2) \exp\left\{\pm i\left[kt - \ln\left(1 + \frac{t}{x}\right)\right]\right\}\left[1 + \frac{C_L b^2}{x(x+t)} + \ldots\right]$$

$$\cdot\left[1 + \frac{A_L + a_L}{x} + O(\frac{1}{x^2})\right] .$$

Contributions to this integral come only from the region around $t \approx 0$ since $\exp(-t^2/2b^2)$ is a strongly peaked function. So we can neglect higher order terms in t/x, so that we have

$$g_L^{\pm}(x) \approx \text{const.} i^{-L} \frac{b^2}{2} \exp(\mp \gamma \ln 2) \frac{1}{x}\left[1 + (A_L + a_L)/x + O(\frac{1}{x^2})\right] \cdot$$

$$\cdot \exp\left[\pm i(kx - \gamma \ln 2 kx - L\pi/2 + \delta_L)\right] \cdot \int_{-\infty}^{+\infty} dt \exp\left[-\frac{t^2}{2b^2} \pm it(k - \frac{\gamma}{x})\right]$$

$$= \text{const.} i^{-L} \frac{b^2}{2} \exp(\mp \gamma \ln 2) \frac{1}{x}\left[1 + (A_L + a_L)/x + O(\frac{1}{x^2})\right] \cdot$$

$$\exp\left[\pm i(kx - \gamma \ln 2 kx - L\pi/2 + \delta_L)\right] \cdot \exp\left[\frac{b^2}{2}(k - \frac{\gamma}{x})^2\right] \cdot \sqrt{2\pi} \cdot b$$

By expanding $\exp\left[\frac{b^2}{2}(k - \frac{\gamma}{x})^2\right] = \exp\left[\frac{b^2}{2}k^2\right]\left(1 - \frac{b^2 \gamma k}{x} + \ldots\right)$ one sees that the correction coefficient $a_L = b^2 \gamma k \equiv b^2 Z_1 Z_2 e^2 u/\hbar^2$ and the ansatz for $f_L(r)$ in fact reproduces $g_L(x)$ up to terms $O(1/x^2)$.

The term $b^2 \gamma k/x$ provides an estimate where to divide the parameter space into an interaction region and an asymptotic region. In the interaction region one solves the Hill-Wheeler equation with the boundary condition that f_L becomes a Coulomb function in the asymptotic region. Neglecting the Coulomb force, de Takacsy [40] was able to make such a division of parameter space at a radius r_o of a few fermi. First numerical tests for $L = o$ indicate that a larger radius r_o is required in the presence of Coulomb forces.

4.3. Prospective applications

There is a small number of applications of GCM in nuclear scattering, most of them on simple systems. Giraud, Hocquenghem and Lumbroso [38] have performed an explicit calculation for elastic scattering of two dineutrons. In this case all kernels in the Lippmann-Schwinger equation can be calculated analytically; this allows to follow what is going on in all phases of the calculation.

Tabakin [43] used the generator function of the type (4.8) in order to study the properties of the effective nucleus-nucleus potential in α-α scattering, if the α-particle has the freedom to adjust its size during collision.

De Takacsy [40] studied α-α and ^{2}n-^{2}n scattering, with the Coulomb potential neglected, by using the first direct method described in Ch. 4.2.2. The phase shifts in ^{2}n-^{2}n scattering were quite the same as those calculated by Giraud, Hocquenghem and Lumbroso [38] in spite of the troubles with the convergency of f if one increases the number of mesh points r_i.

In this chapter we collected a few examples and ideas of the prospective applications of GCM which were discussed during the Seminar. We hope that some of these ideas will prove useful.

4.3.1. α-^{12}C scattering - an approximate projection of fragment spin

In the multipole expansion presented in Sec. 4.2.3. the projection of angular momentum is performed when both scattering nuclei have zero spin. Calculation of kernels, eq. (4.33) , is, however, rather simple only if the scattering nuclei are closed shell nuclei (e.g. ^{4}He, ^{16}O) and if they are in the ground state. In that case, the 0^+ ground state can be approximated by one Slater determinant. The calculation is much more difficult if the wave functions of scattering nuclei correspond to deformed nuclei. In order to get the experimentally relevant phase shifts, each fragment must have a good angular momentum asymptotically. Therefore one has to perform three projections (for each fragment and for the total angular momentum) what is quite unfeasible for nowadays computer abilities. For these reasons we have to limit ourselves to some special situations, in which the projection is still tractable.

One example on the limit of todays possibilities is the α-^{12}C scattering where the ^{12}C ground state may be described by a superposition of few configurations of the α-cluster model. In the following, we limit ourselves to the ground state of ^{12}C which is described by the triangle configuration only. The generator function is then

$$\Phi_o(x_i,r) = \int d\Omega . R_c(\Omega)\Phi(x_i,r) \qquad (4.41)$$

where the operator $R_c(\Omega)$ rotates the three clusters forming the ^{12}C triangle around the centroid of this triangle. This would then ensure that the ^{12}C part of the trial function is a spin zero state and that asymptotically L of Sec. 4.2.3. labels the angular momentum of relative motion.

In all practical calculations one will approximate the integral in (4.41) by a finite sum

$$\Phi_o(x_i,r) \sim \sum_{d=1}^{n} a_d\Phi_d(x_i,r) \ , \qquad (4.42)$$

where the index d labels different orientations of the ^{12}C nucleus relative to the axis connecting the two scattering nuclei.

Note: In a simple one channel calculation one will have to evaluate matrix elements of the type $\langle\Phi_d(x_i,r)|\Phi_{d'}(x_i,r')\rangle$ and $\langle\Phi_d(x_i,r)|H|\Phi_{d'}(x_i,r')\rangle$ for all d and d'. There will be no additional programming work in a coupled channel calculation based on n states

$$\Phi_c(x_i,r) = a_{cd}\Phi_d(x_i,r) \ . \qquad (4.42')$$

There are two alternatives how to choose the coefficients a_d (or a_{cd}):

(i) One may choose the coefficients so that the linear combi-

nations (4.42) (or (4.42')) correspond to definite J=0, apart from a possible admixture of high J components of ^{12}C. in that case one takes the numbers a_{cd} such that they satisfy the equations

$$\sum_d a_{cd} Y_J(\theta_d) = 0 \ , \ J = 1,2,\ldots, n \ .$$

The values of a_{cd} depend on the choice of the discrete set θ_d.

(ii) The coefficients a_{cd} could be chosen so that the Hamiltonian H is asymptotically diagonal in each channel c. In the case of $\alpha + {}^{12}C$ scattering this would simply mean that the a_{cd} are solutions of the eigenvalue problem:

$$\sum_{d'=1}^{n} (\langle\phi_{Bd}|H_B|\phi_{Bd'}\rangle - E_c\langle\phi_{Bd}|\phi_{Bd'}\rangle)a_{cd'} = 0 \qquad (4.43)$$

where the index B denotes that the wave functions ϕ and the Hamiltonian refer to the internal motion of the ^{12}C nucleus.

If the $\Phi_d(x_i,r)$ have the form (4.1) with a relative wave function of the form (4.2)then the new trial states labelled by the channel index c have the same form (4.1). Namely, the width parameters β_d must all be equal because a rotation of the fragment nucleus will asymptotically not affect the relative motion part of the wave function. Additionally, the wave functions $\Phi_d(x_i,r)$ all fulfill the condition (4.29) (because the different orientations labelled by "d" are defined relative to the axis connecting the two nuclei) and the superposition coefficients a_{cd} are independent of the orientation of r. This means that the new trial states $\Phi_c(x_i,r)$ also fulfill condition (4.29) and that the angular variables of r (resp. of q) may be treated in the same way as in Sec. 4.2.3.

The superposition (4.42) corresponds to an approximate projection of the internal angular momentum of the colliding nuclei: for the lowest eigenvalue of eq. (4.43) we obtain the

entrance channel corresponding to two spin-zero fragments. For this channel the quantum number L for total angular momentum asymptotically labels the angular momentum of relative motion of the two nuclei. So in order to calculate the phase shifts δ_L for elastic scattering we have to solve the coupled channel equations (4.31) or (4.36) with the corresponding boundary conditions.

The superpositions (4.42) corresponding to other than the lowest solutions of the eq. (4.43) will correspond to different excited states of the ^{12}C nucleus after the collision. Namely, if the sum (4.42) has only a few components, the approximation will soon become poor as the fragment spin increases. Therefore we cannot proceed with the calculation of phase shifts using the formalism described in Sec.4.2.3, because it is valid only for fragments with zero spin.

A work is now in progress [47] to calculate kernels (4.43), to solve the Lippmann-Schwinger equation and to obtain phase shifts by using the trial function (4.41).

4.3.2. Directional channels

In direct reactions and direct scattering, the differential cross-section often varies strongly with the scattering angle θ. Therefore, too many partial waves would be needed in the multipole expansion and it is preferable to calculate the scattering amplitude directly as a function of angle. A commonly used approximation for this purpose is the (Distorted Wave) Born Approximation. The aim of the present note is to show that in the framework of GCM one can keep the simple general idea of the Distorted Wave Born Approximation, but one can use a more consistent interaction.

Let us introduce the concept of "directional channels" by using $r = |r|$ as a generator coordinate and interpreting θ and ϕ as additional channel lebels. So the channel $c \equiv (t,\theta,\phi)$ is

defined by the reaction type t and the direction (θ,ϕ),(see Fig.4.2).

$$\Phi_c(x_i,r) = \Phi_{CM}\,\mathcal{A}\left[G((r\cos\theta e_z + r\sin\theta\cos\phi\, e_x + r\sin\theta\sin\phi\, e_y - x)^2)\right.$$

$$\left.\Phi_{Ac}(x_i')\Phi_{Bc}(x_j')\right]$$

The directional channels are coupled. If one considers in the trial function sufficient number of properly chosen channels corresponding to directions (θ_d,ϕ_d) the problem is almost equivalent to taking all partial waves in the partial wave expansion. The partial waves have the advantage of being "eigenchannels", while the directional channels have the advantage to provide the amplitude in a chosen direction (without summing up a badly converging series of partial waves).

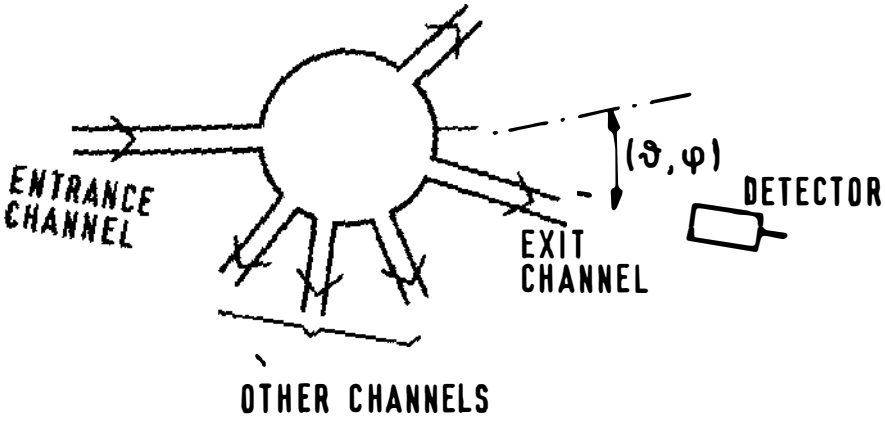

Fig. 4.2. A schematic picture of the "directional" channels.

If one considers only one entrance directional channel and one exit directional channel and decouples all other directions, one gets the GCM generalization of Born Approximation. One has

similar asymptotic wave function as in Born Approximation (apart from $G(r-x)$, eq. (4.1)) and the amplitude function $f(r)$ is allowed distortion in the inner region like in the Distorted Wave Born Approximation. The "potential well" is, however, calculated fully microscopically, eq. (4.24), with $c_1 = (t_1,0,0)$ and $c_2 = (t_2,\theta,0)$.

To go beyond the GCM-Born Approximation one may choose a finite discrete set of channels $c_d \equiv (t,\theta_d,\phi_d)$ around and between the incident direction (0,0) and the "detector direction" $(\theta,0)$. One then solves the Hill-Wheeler equation. The validity and physical relevance of this approximation is still an open problem.

4.3.3. A model for the "adiabatic" scattering and the decay

In Ch. 4.1. we discussed the form of wave function needed in order to describe the "adiabatic" scattering and the decay. Now we shall try to adapt the generator coordinate formalism for the reaction based on a two center shell model (or a constrained Hartree-Fock) determinant. In the following we shall discuss some problems related to the use of the wave function of the type (4.7).

1. Choice of the generator function. We start with an A+B particle determinant

$$\Phi^{D}_{A+B}(x_\ell,\alpha,\beta) \equiv \mathrm{Det}_{A+B} \| \psi_n(x_\ell,\alpha,\beta) \| \qquad (4.44)$$

where single-particle functions ψ_n are defined in this way:

(i) $\phi^{\ell}_i(x-\alpha)$ and $\phi^{d}_i(x-\beta)$ are single particle functions in left and right (harmonic) potentials in fig. 4.3. with centers α and β, respectively.

(ii) $\psi_n(x,\alpha,\beta)$ is a single particle function of the form

$$\psi_n(x,\alpha,\beta) = \sum_{i=1}^{N_\ell} L_{ni}(r)\, \phi^{\ell}_i(x-\alpha) + \sum_{j=1}^{N_d} D_{nj}(r)\, \phi^{d}_j(x-\beta) \qquad (4.45)$$

where $r = |\alpha-\beta|$, and N_ℓ and N_d express the chosen dimension of the single particle basis $\{\phi_i\}$.

The coefficients $L_{ni}(r)$ and $D_{nj}(r)$ are determined by diagonalizing the Hamiltonian with a potential as in Fig.4.3 in the basis $\{\phi_i\}$ and by taking the A+B lowest single particle functions ψ_n.

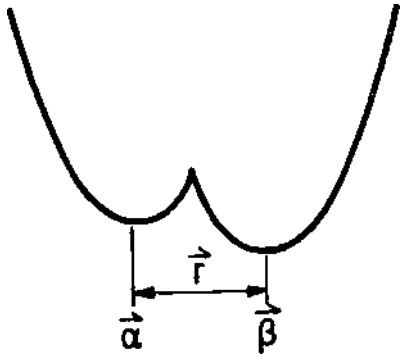

Fig. 4.3 An example of two-center potential for the model of the "adiabatic" scattering

As the next step we form the generator function in this way

$$\Psi_{A+B}(x_\ell,q,p_A,p_B) = \int d^3\alpha \int d^3\beta\, e^{ip_A\alpha}\, e^{ip_B\beta} \cdot \mathcal{A}\left[e^{i(q-p_A)x_A}\, e^{-i(q+p_B)x_B}\, \Phi_{A+B}(x_\ell,\alpha,\beta)\right] \tag{4.46}$$

and we use the trial function

$$\Psi(x_\ell) = \Phi_{CM} \iiint d^3q\, d^3p_A\, d^3p_B\, f(q,p_A,p_B)\Phi_{A+B}(x_\ell,q,p_A,p_B) \tag{4.47}$$

The class of generator coordinate functions (4.46) has the same number of generator parameters as that of Wong, eq. (4.5), but it is more general, because it contains an additional freedom expressed through equation (4.45): It allows to have a different single particle basis for different values of the interpotential

distance r. This freedom is necessary for the decay of a nucleus into two fragments (fission), because at the beginning the decaying nucleus is in the ground state. For the nuclear reactions, the usefulness of the generator function (4.46) depends on the energy and, probably, on the nature of scattering nuclei.

The generator function (4.46) is more complicated than the one of (4.5). The latter can be written in terms of a single Slater determinant, while the function (4.46) is a sum of such determinants. Namely, due to the fact that the Slater determinant (4.44) is antisymmetric, the part of eq. (4.46) with antisymmetrizer $\mathcal{A}$ can be written as follows

$$\mathcal{A}\left[e^{i(q-p_A)x_A}\, e^{-i(q+p_B)x_B}\, \Phi_{A+B}(x_\ell,\alpha,\beta)\right] =$$

$$= \left(\mathcal{S}\left[e^{i(q-p_A)x_A}\, e^{-i(q+p_B)x_B}\right]\right) \Phi_{A+B}(x_\ell,\alpha,\beta) \ ,$$

because $\Phi_{A+B}(x_\ell,\alpha,\beta)$ is a Slater determinant. The symmetrizing operator $\mathcal{S}$ applied to the product of exponential functions gives

$$\mathcal{S}\left[\prod_{i=1}^{A} e^{i(q-p_A)x_{i/A}} \prod_{j=1}^{B} e^{-i(q+p_B)x_{j/B}}\right] =$$

$$= \sum_{\nu=1}^{N_s} \mathcal{P}_\nu(i_A,j_B)\, e^{i(q-p_A)x_{i/A}}\, e^{-i(q+p_B)x_{j/B}} \ ,$$

where $\mathcal{P}_\nu(i_A,j_B)$ is the operator which interchanges the i-th particle in the nucleus A with the j-th particle in the nucleus B. The number of terms is $N_s = \binom{A+B}{A} = \binom{A+B}{B}$ if all A nucleons in the nucleus A and all nucleons in the nucleus B are alike. For example for $^2n + {}^2n$ scattering there are $N_s = 6$ combination. As the nuclei consist of different particles, the determinant $\Phi_{A+B}(x_\ell,\alpha,\beta)$ splits into a product of smaller determinants, and one has to symmetrize only between alike nucleons. (For example, for $\alpha+\alpha$ scattering, the function

$\delta\left[e^{i(q-p_A)x_A}\, e^{-i(q+p_B)x_B}\, \Phi_{A+B}(x_\ell,\alpha,\beta)\right]$ is *one* 4x4 Slater determinant). So the price for the generalization introduced through the class (4.46) is, that we have in general a sum of determinantal functions,

$$\left[\sum_{\nu=1}^{N_S} \mathcal{P}_\nu(i_A,j_B)\, e^{i(q-p_A)x_i/A}\, e^{-i(q-p_B)x_j/B}\right]\Phi_{A+B}(x_\ell,\alpha,\beta) \qquad (4.48)$$

instead of one determinantal function corresponding to the generator function (4.5). This price is not, however, very high, it does not require any additional programming except one "DO" - loop.

2. *Calculation of the kernels* $\langle\Phi_{A+B}(x_\ell,q,p_A,p_B)|\Phi_{A+B}(x_\ell,q',p'_A,p'_B)\rangle$ and $\langle\Phi_{A+B}(x_\ell,q,p_A,p_B)|H|\Phi_{A+B}(x_\ell,q',p'_A,p'_B)\rangle$ between the determinantal functions in (4.48) is similar to those for determinantal functions (4.5) proposed by Wong. In both cases an exact calculation looks impossible for realistic systems and one has to look for reasonable approximations. In practical calculations one will take harmonic oscillator functions for $\phi^{\ell,d}$ in eq. (4.45). In that case it would be possible to perform analytically a significant part of the calculation [42] of the overlap and Hamiltonian kernels. Also, it would be necessary to introduce further approximations, for example by discarding the internal degrees of freedom offered by varying parameters p_A and p_B.

3. *Solution of Lippmann-Schwinger equation* for the trial function (4.47) follows the pattern described in Sec.4.2.3. However, the following warning is necessary: while the function of the type (4.1) allows to separate out the channel energy E_c, eq. (4.10), in the whole range, the present formalism allows such a separation only in the asymptotical region. This has the consequence that w_c, eq. (4.27), is defined as a difference between two large quantities $\langle H\rangle - E_c$ and some caution is required.

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