Generator Coordinate Method for Scattering: An Exact Solution

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An analytically soluble model is given for which an exact numerical solution of the Hill-Wheeler equation in the continuum can be calculated. Properties of this model, which concern in particular the effects of the Pauli principle and the microscopic definition of an optical potential, are considered.

I. INTRODUCTION

It is well known that one of the first physical phenomena for the description of which the generator-coordinate formalism was invented by Griffin, Hill, and Wheeler[1] was this very peculiar nuclear reaction called fission. Actually, for many years the formalism was applied to bound-state problems only, such as nuclear rotations with[2] or without[3] axial symmetry or the study of nuclear shapes and collective motions in light nuclei.[4] In the last few years a fundamental reappraisal of this formalism was made by Jancovici and Schiff,[5] Brink and Weiguny,[6] and Wong[7] and revealed how powerful and general this method was. The elaboration of a generator-coordinate theory of nuclear reactions was undertaken and revived by several authors,[8-17] and it is gratifying that a first success has been achieved with their discoveries of not one, but several, quite different solutions of the Hill-Wheeler equation. One must notice, however, that these solutions have been used only in the case of collisions between (very) light nuclei and that the ultimate aim (namely a microscopic theory of collisions between heavy ions and of fission) is not likely to be reached without suitable approximations in order to avoid enormous calculations.

As in most generator-coordinate problems, three main questions may be asked:
(i) What generator coordinates are relevant to the problem?
(ii) What generating functions must be labeled by these generator coordinates?
(iii) How should the Hill-Wheeler equation be solved?

A. Choice of the Generator Coordinates

There is no doubt that the distance between colliding nuclei is here the most important degree of freedom and this consideration decides the choice of the first generator coordinate. As shown by Wong,[16] complete Galilean invariance for the most general calculation [no factorized center-of-mass wave function as in Eq. (3)] would demand the use of additional coordinates corresponding to an acceleration of the clusters. It is also most tempting to take in account other degrees of freedom[11, 16] such as the deformation of the clusters if they polarize each other during collision or the decompression of the "compound" nucleus in order to correct for the unrealistic prompt[18] limit at low energies. Also the question of complex[6, 13, 16] generator coordinates arises. In view of the difficulties which yet pave the way to a reliable solution of the Hill-Wheeler equation in most cases, it seems that the present status of the theory is more adapted to calculations with one generator coordinate only. (We do not count the case of generator coordinates which correspond to the restoration of a broken symmetry as an additional unreasonable task.) In order to gain a better understanding of the nuclear reactions in the interaction region, we thus advocate, in general, keeping the separation distance as the only generator coordinate and increasing the dimensions of the generator-coordinate subspace by either a set of discrete configurations of the "compound" nucleus or the coupling of various channels.

B. Choice of the Generating Functions

We want to specify a set of wave functions Φ_r, depending on a continuous vector label r (the generator coordinate) and describing two nuclei (A) and (B) at this relative distance r. The aim of the formalism is then to find the many-body wave function,

$$\Psi = \int dr\, f(r)\Phi_r \,, \tag{1}$$

which, by a suitable choice of the Hill-Wheeler amplitude $f(r)$, describes the scattering of these clusters.

Since by definition the interaction region ($|r| <$ a few times b) breaks Galilean invariance for the relative motion, the choice of Φ_r in this latter region is more a matter of nuclear dynamics (two-center shell model,[18] constrained Hartree-Fock,[19] ...) than of kinematics. In the asymptotic region, Galilean invariance for each nucleus can always

be obtained in principle by means of a projection operator[20] for any nucleus (A) with any internal structure ψ^{int}, giving then for the wave function of (A)

$$\Psi_A = \pi^{-3/4}\left(\frac{b}{\sqrt{A}}\right)^{-3/2} \times \exp\left(-\frac{A[R_A - Br/(A+B)]^2}{b^2}\right)\psi^{\text{int}}(\xi_A),$$

where A and B are the nucleon numbers of nuclei (A) and (B). This might give prohibitive configuration mixings, however, if harmonic-oscillator orbitals cannot be used because of $\psi^{\text{int}}(\xi)$. The double projection method of Wong[16] for the extraction of invariant nucleus structure might then be much better. Then if we take for Φ_r the antisymmetrized product of Ψ_A and Ψ_B we keep Galilean invariance of the relative motion in the asymptotic region (large r).

C. Solutions of the Hill-Wheeler Equation

Among the solutions which have been proposed we may quote the following: (i) a boundary condition constraint method[9]; (ii) a direct, discretized solution in coordinate space[12]; (iii) a soluble model in coordinate space.[14]

Only in the first solution were Coulomb effects included. Solutions (i) and (ii) concern f. The last solution concerns a function g (which in the asymptotic region becomes identical with the relative-motion wave function), and gives detailed understanding of the effective potential and the effects of antisymmetrization, at least for simple cases where the formal expressions can be obtained (for instance when the one-particle basis and the potential are Gaussian). A choice between these solutions might be easier if the calculation of the kernels could be simplified, for instance by an omission of possibly weak terms due to core nucleons (or exchange terms) or by a suitable parametrization of these kernels.

The purpose of the present paper is to present a soluble model in momentum space and to discuss some of the physical insight that this formalism provides. The basic formalism is presented in Sec. II. Discussions and proposals for approximations are given in Sec. III. Section IV is our conclusion.

II. BASIC FORMALISM AND ILLUSTRATIVE EXAMPLE OF AN EXACT SOLUTION

In this section, we recall with some detail the analytical illustrative example of Ref. 10. The example is a system of twice two neutrons (dineutron) in an elastic collision. The simplicity of the system allows us to describe the basic formalism without too much complication and it seems to us an easier way to make things comprehensible.

A. Basis $\Phi_{\vec{r}}$

The simplest case which is interesting for us as a significant illustrative example of our theory corresponds to

$$\Phi_{\vec{r}} = \sqrt{6}\,\mathcal{A}_{12,34}\left[\sqrt{2}\,\mathcal{A}_{12}\pi^{-3/2}b^{-3}\exp\left(-\frac{(\vec{r}_1-\vec{r}/2)^2+(\vec{r}_2-\vec{r}/2)^2}{2b^2}\right)\chi_1^+\chi_2^-\right] \times\left[\sqrt{2}\,\mathcal{A}_{34}\pi^{-3/2}b^{-3}\exp\left(-\frac{(\vec{r}_3+\vec{r}/2)^2+(\vec{r}_4+\vec{r}/2)^2}{2b^2}\right)\chi_3^+\chi_4^-\right]. \tag{2}$$

The first bracket in Eq. (2) is the wave function of a cluster (A) made of two neutrons with coordinate vectors $\vec{r}_1$ and $\vec{r}_2$ and spin functions χ_1 and χ_2 (χ^+ and χ^- correspond to spin up and down, respectively). The spatial wave functions for both these neutrons are Gaussian wave packets (of length b) which are centered about the point with coordinate vector $\vec{r}/2$. The second bracket has obviously the same meaning, except that the second cluster (B) is centered about $-\vec{r}/2$. Each cluster is antisymmetrized by means of the proper operator, for instance here $\mathcal{A}_{12} = \frac{1}{2}(1 - P_{12})$, where P_{12} exchanges nucleons 1 and 2. Complete antisymmetry between both clusters is obtained through the usual operator $\mathcal{A}_{12,34} = \frac{1}{6}(1 - P_{13} - P_{14} - P_{23} - P_{24} + P_{13}P_{24} + P_{14}P_{23})$.

B. Relation with the Resonating Group Method

The first bracket in Eq. (2) can be rewritten as

$$\pi^{-3/4}\left(\frac{b}{\sqrt{2}}\right)^{-3/2}\exp\left(-\frac{\vec{R}_A-\vec{r}/2}{b^2}\right)^2\psi_A^{\text{int}}(\vec{\xi}_A), \tag{3}$$

where $\vec{R}_A$ is the center-of-mass coordinate, $\vec{R}_A = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$, and ψ_A^{int} depends only on the internal coordinate $\vec{\xi}_A = \vec{r}_1 - \vec{r}_2$. The same property holds of course for the second bracket if we replace $\vec{R}_A$, ψ_A^{int}, and $\vec{\xi}_A$ by $\vec{R}_B$, ψ_B^{int}, and $\vec{\xi}_B$. If we now reduce $\vec{R}_A$ and $\vec{R}_B$ to their relative coordinate $\vec{\rho} = \vec{R}_A - \vec{R}_B$ and center-of-mass coordinate $\vec{R} = \frac{1}{2}(\vec{R}_A + \vec{R}_B)$, we find

$$\Phi_{\vec{r}}^{\dagger} = \pi^{-3/4}\left(\frac{b}{2}\right)^{-3/2} \exp\left(-\frac{2R^2}{b^2}\right)\sqrt{6}\ \mathcal{A}_{12,34}\Gamma(\vec{\rho},\vec{r})\psi_A^{\text{int}}(\vec{\xi}_A)\psi_B^{\text{int}}(\vec{\xi}_B) \tag{4}$$

with

$$\Gamma(\vec{\rho},\vec{r}) = \pi^{-3/4}b^{-3/2}\exp\left(-\frac{(\vec{\rho}-\vec{r})^2}{2b^2}\right). \tag{5}$$

In this equation (4) we notice that the total center of mass is in a Gaussian wave packet (i) centered about the origin, (ii) obviously a state with zero angular momentum, (iii) independent of $\vec{r}$.

The formalism is thus Galilean invariant and we can forget the center of mass (c.m.) in the following.

We also notice in Eqs. (4) and (5) that the dynamical distance coordinate $\vec{\rho}$ between the two clusters fluctuates in a wave packet about the generator coordinate $\vec{r}$. This was indeed expected from the definition of $\Phi_{\vec{r}}^{\dagger}$. At short distances, however, the physical meaning of $\vec{r}$ becomes ill-defined because of the antisymmetrization. This question of antisymmetrization will be considered in subsection II D.

If we now insert Eqs. (4) and (5) into Eq. (1) we find

$$\Psi = \text{c.m.}\sqrt{6}\ \mathcal{A}_{12,34}g(\vec{\rho})\psi_A^{\text{int}}(\vec{\xi}_A)\psi_B^{\text{int}}(\vec{\xi}_B) \tag{6}$$

with

$$g(\vec{\rho}) = \int d\vec{r}\,\Gamma(\vec{\rho},\vec{r})f(\vec{r}). \tag{7}$$

We recognize that the function $g(\vec{\rho})$ is the usual scattering (or possibly bound) wave and that our formalism is equivalent to the resonating group method (RGM).[21] As we show in the next subsection, however, the generator-coordinate formulation of scattering might lead to calculations easier than those of the RGM, for it is never necessary to use relative coordinates $\vec{\rho}$, $\vec{\xi}_A$, $\vec{\xi}_B$. All calculations can be performed with the single-nucleon coordinates $\vec{r}_1$, $\vec{r}_2$, ...

C. Hill-Wheeler Equation

It is now convenient to rewrite Eq. (2) in second quantization. This is trivial because $\Phi_{\vec{r}}^{\dagger}$ is a Slater determinant, and this can be generalized by means of suitable translation operators if clusters (A) and (B) must be described by configuration mixings. In the present case, we define the creation operator $a_{\pm}^{\dagger}(\vec{y})$ of a neutron with spin up (down) in a Gaussian wave packet of length b centered about the point of vector coordinate $\vec{y}$, and we obtain

$$|\Phi_{\vec{r}}^{\dagger}\rangle = a_{-}^{\dagger}\left(-\frac{\vec{r}}{2}\right)a_{+}^{\dagger}\left(-\frac{\vec{r}}{2}\right)a_{-}^{\dagger}\left(\frac{\vec{r}}{2}\right)a_{+}^{\dagger}\left(\frac{\vec{r}}{2}\right)|0\rangle, \tag{8}$$

where $|0\rangle$ is the vacuum.

Our Hamiltonian H contains the kinetic energy of all nucleons and a two-body potential $\sum_{i<j} V_{ij}$, where

$$V_{ij} = U_0\exp\left(-\frac{(\vec{r}_i-\vec{r}_j)^2}{\mu^2}\right)(A + BP_\sigma + CP_\tau + DP_\sigma P_\tau). \tag{9}$$

In Eq. (9), U_0 is the potential depth, μ is the range, P_σ and P_τ are exchange operators for spin and isospin, and A, B, C, D give the corresponding exchange mixture.

We take advantage of Eq. (8) to calculate the kernels

$$H(\vec{r},\vec{r}') = \langle\Phi_{\vec{r}}^{\dagger}|H|\Phi_{\vec{r}}^{\dagger\prime}\rangle \tag{10a}$$

and

$$N(\vec{r},\vec{r}') = \langle\Phi_{\vec{r}}^{\dagger}|\Phi_{\vec{r}}^{\dagger\prime}\rangle \tag{10b}$$

of the Hill-Wheeler equation. The second-quantization technique we used is that of Löwdin[22] and has al-

ready been used by many authors. We thus find the overlap operator

$$N(\vec{r},\vec{r}\,') = \left[\exp\left(-\frac{(\vec{r}-\vec{r}\,')^2}{8b^2}\right) - \exp\left(-\frac{(\vec{r}+\vec{r}\,')^2}{8b^2}\right)\right]^2 . \tag{11}$$

As regards the Hamiltonian kernel $H(\vec{r},\vec{r}\,')$, we can take into account the fact that only the *relative* energy between the clusters is of interest in the formalism. It is then necessary to subtract from the total energy of this four-nucleon system:
(i) the internal energy of each cluster, namely, if we call the nucleon mass m, $T^{\text{int}} = \frac{3}{4}\hbar^2/(mb^2)$ for the kinetic energy and, as it can be shown in a trivial calculation, $V^{\text{int}} = 2U_0(A-B+C-D)(1+2b^2/\mu^2)^{-3/2}$ for the potential energy;
(ii) the kinetic energy of the total center of mass, $T^{\text{c.m.}} = \frac{3}{4}\hbar^2/(mb^2)$.
If thus we subtract from the Hamiltonian kernel the quantity $(2T^{\text{int}} + 2V^{\text{int}} + T^{\text{c.m.}})N(\vec{r},\vec{r}\,')$, the eigenvalue E which is left in the Hill-Wheeler equation is the relative kinetic energy $(\hbar^2k^2)/(2m)$ between the two clusters (where k is the relative wave number). The new Hamiltonian kernel H' is then the sum of a kinetic-energy part,

$$T(\vec{r},\vec{r}\,') = \frac{\hbar^2}{mb^2}\left[\exp\left(-\frac{(\vec{r}-\vec{r}\,')^2}{8b^2}\right) - \exp\left(-\frac{(\vec{r}+\vec{r}\,')^2}{8b^2}\right)\right]$$
$$\times\left\{\left[\frac{3}{4} - \frac{(\vec{r}-\vec{r}\,')^2}{8b^2}\right]\exp\left(-\frac{(\vec{r}-\vec{r}\,')^2}{8b^2}\right) - \left[\frac{3}{4} - \frac{(\vec{r}+\vec{r}\,')^2}{8b^2}\right]\exp\left(-\frac{(\vec{r}+\vec{r}\,')^2}{8b^2}\right)\right\}, \tag{12}$$

and of a potential-energy part,

$$V(\vec{r},\vec{r}\,') = 2U_0(1+2b^2/\mu^2)^{-3/2}\times 2(A-B+C-D)\exp\left(-\frac{r^2+r'^2}{4b^2}\right)\left[1-\exp\left(-\frac{r^2}{8b^2+4\mu^2}\right)-\exp\left(-\frac{r'^2}{8b^2+4\mu^2}\right)\right]$$
$$+(2A+B+2C+D)\left[\exp\left(-\frac{(\vec{r}+\vec{r}\,')^2}{8b^2+4\mu^2}\right)\exp\left(-\frac{(\vec{r}-\vec{r}\,')^2}{4b^2}\right)+\exp\left(-\frac{(\vec{r}-\vec{r}\,')^2}{8b^2+4\mu^2)}\right)\exp\left(-\frac{(\vec{r}+\vec{r}\,')^2}{4b^2}\right)\right]$$
$$-(A+2B+C+2D)\exp\left(-\frac{\vec{r}^{\,2}+\vec{r}\,'^2}{4b^2}\right)\left[\exp\left(-\frac{(\vec{r}+\vec{r}\,')^2}{8b^2+4\mu^2}\right)+\exp\left(-\frac{(\vec{r}-\vec{r}\,')^2}{8b^2+4\mu^2}\right)\right]. \tag{13}$$

We point out that for large values of $\vec{r}$ and (or) $\vec{r}\,'$, the kernels N, T, V have the following properties:
(i) $N(\vec{r},\vec{r}\,')$ becomes Gaussian, and actually $N \approx \Gamma^2$;
(ii) $T(\vec{r},\vec{r}\,')$ also fulfills the Gaussian overlap and quadratic-approximation conditions,[6] and the kinetic energy $\frac{3}{4}\hbar^2/(mb^2)$ due to the zero-point relative motion coexists with significant negative-energy contributions due to the *nonlocality* of this kernel (indeed the limit $\mathcal{T}$ of T in the region depends only on $\vec{x} = \vec{r} - \vec{r}\,'$ and $\int \mathcal{T}(\vec{x})\, d\vec{x} = 0$);
(iii) $V(r,r')$ is negligible.

D. Exact Solution

Given the Hill-Wheeler equation

$$\int d\vec{r}\,'\,[T(\vec{r},\vec{r}\,') + V(\vec{r},\vec{r}\,') - EN(\vec{r},\vec{r}\,')]f(\vec{r}\,') = 0, \tag{14a}$$

or, in operator notation

$$(T+V-EN)f = 0, \tag{14b}$$

we can reduce it to an operator diagonalization problem by two methods, namely the following transformed equations: either

$$[N^{-1/2}(T+V)N^{-1/2} - E](N^{1/2}f) = 0, \tag{15}$$

or

$$[(T+V)N^{-1} - E](Nf) = 0. \tag{16}$$

By definition [Eq. (10b)] the kernel N is nonnegative and therefore $N^{1/2}$ is well defined. But there might arise difficulties in either method, for the inversion of N or $N^{1/2}$ could be singular. In the latter method [Eq. (16)] the operator $(T+V)N^{-1}$ is non-Hermitian. It thus seems preferable to stick to the former, [Eq.

(15)]. Also, from the remark (i) we made just above, concerning the fact that $N \approx \Gamma^2$ in the asymptotic regions (large $\vec{r}$ or $\vec{r}'$), the problem of finding the square root $N^{1/2}$ of the operator N is almost solved by the knowledge of Γ. Finally, in view of Eq. (7), it is clear that it is physically very useful to consider $g = \Gamma f$ as the proper unknown function in our formalism. The corresponding, minor modification of Eq. (15) is thus

$$\Gamma^{-1}(T + V - EN)\Gamma^{-1} g = 0 \tag{17}$$

and this has the further advantage that the boundary conditions for g are the well known conditions for scattering waves, while the prescription of suitable boundary conditions for f may still be considered as an open problem.

The inversion of Γ, however, is not a regular operation in coordinate space. This well-known difficulty is clearly revealed by the Fourier transform

$$\Gamma(\vec{q}, \vec{q}') = \pi^{-3/4} b^{3/2} \exp\left(-\frac{b^2 q^2}{2}\right) \delta(\vec{q} - \vec{q}') \tag{18}$$

which shows that Γ^{-1} diverges at high frequencies. This divergence, however, is compensated by the strong decrease (at high frequencies) of the Fourier transforms of N, T, V;

$$N(\vec{q}, \vec{q}') = (4\pi)^{3/2} b^3 \exp(-b^2 q^2)[\delta(\vec{q} - \vec{q}') + \delta(\vec{q} + \vec{q}')] - 16 b^6 \exp[-b^2(q^2 + q'^2)], \tag{19}$$

$$T(\vec{q}, \vec{q}') = \frac{\hbar^2}{m b^2}\left\{(4\pi)^{3/2} b^3 \frac{b^2 q^2}{2} \exp(-b^2 q^2)[\delta(\vec{q} - \vec{q}') + \delta(\vec{q} + \vec{q}')] - 8 b^6 [b^2(q^2 + q'^2) - \tfrac{3}{2}] \exp[-b^2(q^2 + q'^2)]\right\}, \tag{20}$$

$$\begin{aligned} V(\vec{q}, \vec{q}') = {} & 2U_0 (1 + 2b^2/\mu^2)^{-3/2}\, 2(A - B + C - D)(b\sqrt{2})^6 \\ & \times \left\{ \exp[-b^2(q^2 + q'^2)] - \left(\frac{\beta}{b\sqrt{2}}\right)^3 \left[\exp\left(-\frac{\beta^2 q^2}{2}\right) \exp(-b^2 q'^2) + \exp(-b^2 q^2) \exp\left(-\frac{\beta^2 q'^2}{2}\right)\right]\right\} \\ & + (2A + B + 2C + D)(\alpha b)^3 \left[\exp\left(-\frac{(2b^2 + \mu^2)(\vec{q} - \vec{q}')^2 + b^2(\vec{q} + \vec{q}')^2}{4}\right) + \exp\left(-\frac{b^2(\vec{q} - \vec{q}')^2 + (2b^2 + \mu^2)(\vec{q} + \vec{q}')^2}{4}\right)\right] \\ & - (A + 2B + C + 2D)(\gamma b\sqrt{2})^3 \left\{ \exp\left[-\frac{b^2\alpha^2(\vec{q} - \vec{q}')^2}{2(4b^2 + \mu^2)} - \frac{b^2}{2}(\vec{q} + \vec{q}')^2\right] + \exp\left[-\frac{b^2\alpha^2(\vec{q} + \vec{q}')^2}{2(4b^2 + \mu^2)} - \frac{b^2}{2}(\vec{q} - \vec{q}')^2\right]\right\}, \end{aligned} \tag{21}$$

with

$$\alpha^2 = 2b^2 + \mu^2, \quad \frac{1}{\beta^2} = \frac{1}{2\alpha^2} + \frac{1}{2b^2}, \quad \frac{1}{\gamma^2} = \frac{1}{\alpha^2} + \frac{1}{2b^2}. \tag{21'}$$

No critical divergence is left for the resulting kernels $n = \Gamma^{-1} N \Gamma^{-1}$, $t = \Gamma^{-1} T \Gamma^{-1}$, and $v = \Gamma^{-1} V \Gamma^{-1}$. For instance, we find

$$n(\vec{q}, \vec{q}') = 2(2\pi)^3 \left[\frac{\delta(\vec{q} - \vec{q}') + \delta(\vec{q} + \vec{q}')}{2} - \pi^{-3/4} b^{3/2} \exp\left(-\frac{b^2 q^2}{2}\right) \exp\left(-\frac{b^2 q'^2}{2}\right) b^{3/2} \pi^{-3/4}\right], \tag{22}$$

$$t(\vec{q}, \vec{q}') = 2(2\pi)^3 \frac{\hbar^2}{2m} \left[q^2 \frac{\delta(\vec{q} - \vec{q}') + \delta(\vec{q} + \vec{q}')}{2} - \pi^{-3/4} b^{3/2} \exp\left(-\frac{b^2 q^2}{2}\right)\left(q^2 + q'^2 - \frac{3}{2b^2}\right) \exp\left(-\frac{b^2 q'^2}{2}\right) b^{3/2} \pi^{-3/4}\right]. \tag{23}$$

If we divide all kernels n, t, v by the irrelevant constant $2(2\pi)^3$ and restrict ourselves to even waves $g(\vec{q})$, we can conclude that the final form of Eq. (17) is a Schrödinger equation in momentum representation

$$\left(\frac{\hbar^2}{2m} q^2 - E\right) g(\vec{q}) + \int dq' [\Omega(\vec{q}, \vec{q}') + v(\vec{q}, \vec{q}') + EQ(\vec{q}, \vec{q}')] g(\vec{q}') = 0. \tag{24}$$

E. Calculation of Phase Shifts

After a proper multipole expansion of $g(\vec{q})$ and $w(\vec{q}, \vec{q}')$ (with $w = \Omega + v + EQ$) we write Eq. (24) as (all angular momentum labels omitted)

$$(q^2 - k^2)g(q) + \int_0^\infty dq' w(q, q')g(q') = 0 . \tag{25}$$

The corresponding equation for the reaction matrix is

$$K(q, k) = w(q, k) + \int_0^\infty dq' w(q, q') \frac{P}{k^2 - q'^2} K(q', k), \tag{26}$$

where P denotes a principal-part value. A suitable discretization of the principal-part integral gives

$$K(q_i, k) = w(q_i, k) + \sum_{j=1}^{M} w(q_i, q_j) \frac{\omega_j}{k^2 - q_j^2} K(q_j, k), \quad i, j = 1, M , \tag{27}$$

where the M numbers ω_j are the integration weights related to the M points q_j of the integration mesh. The mesh and weights must of course be adapted to the principal part integration and necessarily $q_j \neq k, \forall j$. The values of the M unknown quantities $K(q_i, k)$ are thus the solutions of a system of M linear equations (27). It is then trivial to derive the "on-shell" reaction matrix $K(k, k)$, whence the phase shift

$$tg\eta(k) = -\frac{\pi}{2k} K(k, k) . \tag{28}$$

For the sake of completeness we reproduce in the table below the results obtained[10] in the S wave with the Brink and Boeker force $B1$,[23] and a size parameter $b = 1.5$ fm, although the choice of Φ_r^τ [Eq. (2)] is physically unrealistic. The energy range, from 0 to 1000 MeV, is also unrealistic when compared to the validity range of our one-channel description of elastic scattering, but it was chosen for a complete check of numerical accuracy:

E (MeV)	0	3	10	20	40	50	60	70	100	200	400	500	1000
η (rad)	3.14	2.2	1.48	0.90	0.30	0.12	−0.02	−0.14	−0.40	−0.83	−1.02	−1.00	−0.79

III. DISCUSSION

Besides the several mathematical properties which have been encountered in the previous section in the process of derivation and solution of the Hill-Wheeler equation, one may notice three main physical aspects: occurrence of the exact reduced mass, effects of the Pauli principle, and calculation of an effective microscopic potential.

It is remarkable that the mass which appears in our final Schrödinger equation (24) is the exact reduced mass. It is clear that this occurrence of the correct reduced mass is due to the fact that Φ_r [Eq. (4)] corresponds to Galilean invariance of the *relative* motion in the *asymptotic* region (large r).

It is often claimed that the way to parametrize the behavior of the colliding system in the interaction region is to use an effective mass (which of course would tend to the reduced mass in the asymptotic region). We have just seen, however, that only the reduced mass appears in the present exact formalism, together with local potentials, nonlocal potentials, and pseudopotentials. The conversion of these *nonlocal* terms into corrections from the reduced mass to an effective mass would amount to replacing square-integrable operators by the presumed correction

$$-\frac{\hbar^2}{2}\left[\frac{1}{m_{\text{eff}}(\rho)} - \frac{1}{m_{\text{red}}}\right]\frac{d^2}{d\rho^2} ,$$

which is no longer square-integrable (nor Hermitian, but a symmetrization is possible). As far as we know, the consequences of this mathematical modifcation of the formalism have not been studied and deserve more attention.

We now turn to the problem of the influence of the Pauli principle on our formalism. A simple inspection of Eqs. (19)–(23) proves that the action of any of the operators N, T, V (n, t, v) upon any odd-parity function $f_{\text{odd}}(q)$ or $g_{\text{odd}}(q)$ gives a vanishing result. This corresponds of course to the fact that we have considered the collision of identical even nuclei. Besides the potential kernel v, Eq. (24) contains two pseudopotentials Ω and Q which are the non-δ-function terms shown by Eqs. (22) and (23). These pseudopotentials are due to exchange matrix elements in the calculation of the kinetic energy and overlap kernels. As shown in Ref. 10 and generalized by Zaikin[15] the role of Q is to take in account the effects of the Pauli principle which remain after we have eliminated the

odd waves g_{odd}. The same role was already known in the framework of the resonating-group method.[24] An inspection of kernel Q reveals that it is a projector $|0s\rangle\langle 0s|$ onto the $0s$ harmonic-oscillator state of relative motion between the colliding di-neutrons. This $0s$ state of relative motion is indeed forbidden by the Pauli principle, as it may be readily seen if one counts the number of oscillator quanta which are present in Φ_r when $r \to 0$ (one must normalize Φ_r to unity in this limit process). The kernel $n = 1 - Q$ is thus the projector onto the waves of relative motion which are allowed by the Pauli principle, namely, in the present case, all even-parity states except for the $0s$. A similar inspection of kernel t [Eq. (23)] reveals that the "forbidden states" by n are also forbidden by t; in other words, there is an operator θ which fulfills the identity $t \equiv (1 - Q)\theta(1 - Q)$. Finally a simple but tedious calculation shows that the potential kernel v has the same property $v \equiv (1 - Q) \times v(1 - Q)$. More details can be found in Zaikin,[15] where this result is extended.

Finally, as regards the validity of an optical potential, several points can be raised. It has been seen above that the transformation of the Hill-Wheeler equation into an equivalent Schrödinger equation leads to an effective potential w, namely the bracket $[\Omega + v + EQ]$ of Eq. (24). This potential is of a great physical interest in itself and may be analyzed either in momentum space or through a Fourier transform back to coordinate space. However, the burden of calculations in realistic cases becomes rapidly prohibitive and one may think of replacing w by an optical potential. In each specific case the detailed analysis of w must allow us to determine which terms are important (for instance it has been shown in Ref. 10 that the exchange terms in n was not) so as to obtain a simplified expression. We can hope that this will lead to prescriptions for calculations of optical potentials.

IV. CONCLUSION

The results which have been achieved may be summarized as follows: transformation of the Hill-Wheeler equation into a Schrödinger equation allowing the calculation of the phase shifts in a simple way, understanding of the Pauli principle effects, obtaining a way of derivation of the optical potential starting from the nucleon-nucleon force.

The next steps which are desirable are clearly the inclusion of coupled waves, nuclear polarizability, and Coulomb effects. They can be obviously included in the present formalism.

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Sum Rules, Random-Phase-Approximation, and Constrained Self-Consistent Fields*

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It is shown that the energy-weighted and inversely-energy-weighted (IEW) random-phase-approximation sum rules may be obtained simultaneously by a doubly constrained self-consistent field calculation. Applications of the IEW sum rule are made to the quadrupole-force Hamiltonian, including a case when zero-frequency modes occur. The relevance to certain higher-order sum rules is noted and discrepancies in some calculations of centrifugal stretching effects in spherical and deformed nuclei are pointed out.

I. INTRODUCTION

The energy-weighted (EW) sum rule in the random-phase approximation (RPA) has been discussed by many authors,[1] but relatively little has been said about the inversely-energy-weighted (IEW) sum rule, which is of importance, for example, in calculating effective charges. The purpose of this note is to fill this gap in the literature. In particular, it will be shown that the IEW sum evaluated with RPA eigenstates is proportional to the reciprocal of a "spring constant" obtained from a constrained self-consistent field (SCF) calculation, in accordance with the interpretation of such sums as polarizabilities. Also, the EW sum may be interpreted as the reciprocal of a conjugate "mass parameter," both sum rules following at once from a doubly constrained SCF calculation. Thus, it is not at all necessary to diagonalize the RPA matrix to evaluate the IEW sum as has been done in some previous work; a perturbed SCF calculation is sufficient.

Examples will be given for a Hamiltonian with separable interaction such as the quadrupole-quadrupole force. The case when zero-frequency modes are present will be illustrated for nuclear rotation. The extension of these ideas to higher-order sum rules will be pointed out, and, in this connection, some shortcomings of previous calculations of static quadrupole moments of vibrational states of spherical nuclei and rotation-vibration coupling effects in deformed nuclei (both may be regarded as centrifugal stretching effects) are noted.

II. EXACT SUM RULES

The exact EW sum rule for any operator $\hat{Q}$ is given by

$$2\sum_k (E_k - E_0)(0|\hat{Q}|k)(k|\hat{Q}|0) = (0|[\hat{Q},[H,\hat{Q}]]|0)\,, \tag{II.1}$$

where $H|k) = E_k|k)$, $|0)$ denoting the ground state of the Hamiltonian H. The IEW sum rule can be obtained from (II.1) by introducing an operator S satisfying the relations

$$(k|[H,S]|0) = (k|\hat{Q}|0)\,, \quad k \neq 0 \tag{II.2}$$

leading to

$$2\sum_{k\neq 0} \frac{(0|\hat{Q}|k)(k|\hat{Q}|0)}{E_k - E_0} = (0|[[H,S],S]|0) = (0|[\hat{Q},S]|0)\,, \tag{II.3}$$