The results of the analysis are shown in Table I. It can be seen that θ_n^2 and S differ by about a factor of 10^3 for $l=1$, but agree to within a factor of 2 for $l=2$.

Adding a $d_{5/2}$ neutron to the ground state of $^{11}B(J^\pi=\frac{3}{2}^-)$ yields possible spins 1, 2, 3, and 4 and negative parity. (A $d_{3/2}$ transfer would have allowed $J=0$, but the $d_{3/2}$ strength is expected to lie several MeV above the $d_{5/2}$ strength. $J=0$ is also independently ruled out by the results of Mooring *et al.*) If the final spin were $J=1$ or 2, the state could be reached via $l=0$ as well as $l=2$. There is no indication of any $l=0$ strength in either the $^{11}B(d,p)$ or the $^{11}B+n$ work. Therefore, the final spin should be either 3^- or 4^-. The γ-decay branching ratio of this state[3] seems to rule out $J=4$, leaving $J^\pi=3^-$ as the most likely assignment consistent with all the data.

In summary, the comparison of reaction and elastic scattering data has yielded an unambiguous assignment of negative parity for the 3.39-MeV state of ^{12}B, in contradiction to the results of earlier analyses.[1,2] The spin assignment is not unique, but combining all the available data for this state leads to $J^\pi=3^-$ as the most likely assignment.

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Comprehensive Formalism for Nuclear-Reaction Problems. III. Calculable Theories with Systematic "Discretization"*

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The comprehensive formalism of earlier papers is specialized in the direction of calculable theories of nuclear reactions especially those based on the shell model such as that of Bloch and Fano. Unlike the basis states used in previous specialization, the shell-model states do not, in general, have the property that $(H+\mathfrak{L})$ is Hermitian. We show that this complication is no real obstacle, and that only a weaker Hermiticity condition is needed. The final result is a number of forms of calculable theories of the R-matrix kind. No continuum-continuum interaction problems exist, since continua do not occur. This and other merits of the results are discussed from the viewpoint of practical calculations.

I. INTRODUCTION

IN the two earlier papers[1,2] (I and II), we have set up a comprehensive theory of reactions based on Bloch's $\mathfrak{L}$ operator,[3] and have specialized this to yield six existing theories (I), and also a theory of line broadening with fine structure (II). Each of the seven theories is characterized by the basis which is used to develop the Green's-function operator, $\mathcal{G}\equiv(H+\mathfrak{L}-E)^{-1}$. The merit of the combination $H+\mathfrak{L}$ is that it facilitates the derivation of results for the scattering matrix, etc. If the set $|p\rangle$ are eigenstates of a Hamiltonian H^0 and satisfy $\mathfrak{L}^0|p\rangle=0$, and if $(H+\mathfrak{L})$ is Hermitian in the states $|p\rangle$,

$$\mathcal{G}=\sum_{p,q}|p\rangle\langle\tilde{p}|\mathcal{G}|q\rangle\langle\tilde{q}|. \tag{1}$$

The term Hermitian for operators like $(H+\mathfrak{L})$ will be used even though $(H+\mathfrak{L})$ is "trivially" non-Hermitian, because of the use of complex boundary conditions, so that $(H+\mathfrak{L})^\dagger=H+\mathfrak{L}^*$. The term non-Hermitian will be used whenever $(H+\mathfrak{L})^\dagger\neq H+\mathfrak{L}^*$. On defining

$$\mathcal{G}^0=(H^0+\mathfrak{L}^0-E)^{-1}, \tag{2}$$

$$h=(H-H^0)+(\mathfrak{L}-\mathfrak{L}^0), \tag{3}$$

then

$$\mathcal{G}=(1+\mathcal{G}^0h)^{-1}\mathcal{G}^0 \tag{4}$$

and the matrix elements $\langle\tilde{p}|\mathcal{G}|q\rangle$ that give the scattering matrix are obtained from the matrix version of Eq. (4), with operators $\mathcal{G}$, $\mathcal{G}^0$, h replaced by their

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[1] A. M. Lane and D. Robson, Phys. Rev. **151**, 774 (1966).
[2] D. Robson and A. M. Lane, Phys. Rev. **161**, 982 (1967).
[3] C. Bloch, Nucl. Phys. **4**, 503 (1957).

matrices. For a particular theory, h has particular properties, which enable the equation to be developed further, and the particular scattering matrix form to be deduced. The main property is whether $H-H^0$ or $\mathfrak{L}-\mathfrak{L}^0$ vanishes. In Table I, this property is listed for the seven previous theories.

The object of the present paper is to use the comprehensive formalism to yield so-called "calculable" theories of reactions based on the shell model. In particular, we have in mind the work of Bloch and Fano. Bloch[4] has adapted to nuclear physics a theory set up by Fano[5] for the calculation of atomic resonance cross sections. This is based on the shell model, i.e., the total wave function is expanded in shell-model states. The theory does not single out an "interaction region" in the configuration space of the particles, but treats all the space without any distinctions. It follows that the single-particle states include continua. This gives rise to problems. First, if the theory is to be antisymmetric, the expansion must be restricted to states with, at most, one continuum particle. This is necessary to avoid ambiguities, and makes the theory approximate. Second, while causing no formal problem, the interaction between those states involving a continuum particle does give rise to a calculational one. In fact, the theory has not been put in an explicit calculable form when this interaction is included. Some useful devices[6,7] which are numerically accurate have been set up. One of these is the "discretization" procedure used by Bloch and Gillet,[6] in which the continua are broken into a finite number of intervals, thereby making them like discrete states. The usual methods of finite matrix inversion and diagonalization then apply. The snag is that certain energy regions (those near single-particle resonances) need to be treated with a much finer mesh than others.

The "calculable" theories of the present paper like those of Tobocman and collaborators[8–10] and the earlier work of Danos and Greiner[11] attempt to avoid these two problems by using the philosophy of Kapur-Peierls[12] and R-matrix[13] theory in which the finite interaction region is treated specially. In fact, the basis states are used only in this region, so that they do not have to involve continua, because a complete set can be made from discrete states alone.

In using the comprehensive formalism to this end, we encounter the problem that the shell-model basis does not, in general, have the property that $(H+\mathfrak{L})$ is Hermitian in it. However, it turns out that this property is unnecessary.

In Sec. II, this matter of non-Hermiticity is demonstrated, and it is shown that this does not impede the expansion of the exact wave function, which is sufficient for development of the scattering matrix. Section III presents various forms of "calculable" theories, while Sec. IV discusses their use in practice, and Sec. V covers a number of issues met when the theories are applied to shell-model states.

II. NON-HERMITICITY OF $H+\mathfrak{L}$ IN STATES $|p\rangle$ AND EXPANSION OF THE WAVE FUNCTION

In the present paper, we are concerned with adding an eighth item to the list of Table I, viz., the class of "calculable" theories based on shell-model states for the set $|p\rangle$. Bloch[4] and Fano's[5] theory comes under this heading, with the special feature that no "interaction" or "interior" region is used. In the $\mathfrak{L}$-operator formalism, this means that the channel radii are taken to infinity. It is straightforward to derive the results of Bloch and Fano in this situation (Appendix A), very much as the results of the MacDonald[14] and Feshbach[15] theories were derived in I. In the limit of large radii, the $\mathfrak{L}$ operator in the combination $(H+\mathfrak{L}-E)^{-1}$ may be replaced[16] by $-i\epsilon$, giving the familiar form $(H-i\epsilon-E)^{-1}$.

In the general case, when the interaction radii are finite, we cannot derive reaction theories in terms of shell-model states with the method used in I and II, because $(H+\mathfrak{L})$ is not Hermitian in these states. It is easy to see this. First, let us be more precise about the "shell-model states." These are products of single-particle states, which are defined by a boundary condition on a certain radius. (In order that the states be complete in the interior region, this radius must be larger than all the channel radii. The absence of a fixed centroid in the shell model is also involved in this condition—see further comments in Sec. V.)

Next, let us recall the structure of the $\mathfrak{L}$ operator:

$$\mathfrak{L}(b)=\sum_c |c\rangle \frac{\hbar^2}{2m_c}\delta(r_c-a_c)\left(\frac{d}{dr_c}-\frac{b_c-1}{a_c}\right)\langle c|. \quad (5)$$

Here, $|c\rangle$ is the channel wave function (including relative angular motion) for the two-body channel c, r_c is the separation of the two fragments of channel c, and a_c is the channel radius. m_c is the channel mass, and b_c is the set of boundary condition constants; b is short-

[4] C. Bloch, in Lectures held at Varenna Summer School, Villa Monastero, Varenna, 1965 (unpublished).
[5] U. Fano, Phys. Rev. **124**, 1866 (1961); U. Fano and F. Prats, in *Proceedings of the National Academy of Science, India* (Council of the National Academy of Sciences, Allalhabad, United Provinces, India, 1963), Sec. A, Vol. 33, p. 553.
[6] C. Bloch and V. Gillet, Phys. Letters **16**, 62 (1965); **18**, 58 (1965).
[7] W. Glockle, J. Hufner, and H. A. Weidenmuller, Nucl. Phys. **A90**, 481 (1967).
[8] L. Garside and W. Tobocman, Phys. Rev. **173**, 1047 (1968).
[9] W. Tobocman and M. A. Nagarajan, Phys. Rev. **138**, 1351 (1965).
[10] M. A. Nagarajan, S. K. Shah, and W. Tobocman, Phys. Rev. **140**, 63 (1965).
[11] M. Danos and W. Greiner, Phys. Rev. **138**, 93 (1965).
[12] P. L. Kapur and P. E. Peierls, Proc. Roy. Soc. (London) **A166**, 277 (1938).
[13] E. P. Wigner and L. Eisenbud, Phys. Rev. **72**, 29 (1947).
[14] W. M. MacDonald, Nucl. Phys. **54**, 393 (1964); **56**, 636 (1964); **56**, 647 (1964).
[15] H. Feshbach, Ann. Phys. (N.Y.) **5**, 357 (1958).
[16] B. A. Robson and D. Robson, Phys. Letters **25B**, 504 (1967).

hand for the set b_c. The operator $\mathfrak{L}$ without argument correspond to outgoing wave conditions

$$b_c=[r_cO_c^{-1}(dO_c/dr_c)]_{rc=ac}, \tag{6}$$

where $O_c(r_c)$ is the outgoing wave solution which approaches $\exp(ik_cr_c)$ as $r_c\to\infty$. Ignoring centroid motion, the shell-model states may be chosen to satisfy $\mathfrak{L}^0\mid p\rangle=0$, where $\mathfrak{L}^0\equiv\mathfrak{L}(b)$, the boundary condition operator with radii a_c, and boundary conditions b_c are equal to the shell-model values.

Despite the fact that the states $\mid p\rangle$ are eigenstates of a Hamiltonian H^0 (the shell-model one) and of $\mathfrak{L}^0$ the combination $(H+\mathfrak{L})$ is not Hermitian in the shell-model basis. The reason is that the surface term arising when Green's theorem is applied to the volume integral $\langle\tilde{p}\mid H\mid q\rangle-\langle\tilde{q}\mid H\mid p\rangle$ is not exactly cancelled by the terms $\langle\tilde{p}\mid\mathfrak{L}\mid q\rangle-\langle\tilde{q}\mid\mathfrak{L}\mid p\rangle$. The difference comes from the presence of unbound channel states c in the shell-model states; these three- (or more-) body states are not included in the sum on c in $\mathfrak{L}$. It is worthwhile at this stage to distinguish between the finite potential and infinite potential shell-model bases. The complete set for the former will always involve configurations with three or more particles in positive energy orbitals which have wave functions that oscillate to infinity. The latter, however, has wave functions which all go to zero at infinity. Consequently, for infinite potentials (e.g., harmonic oscillators), the Hermicity of $(H+\mathfrak{L})$ can be maintained, provided the internal region is chosen to be that bounded by finite-range surfaces for two-body open channels and infinite-range surfaces for three- (or more-) body channels. Such an internal region is physical, provided one is below the thresholds for all three- (or more-) body channels.

Because of the possibility of non-Hermiticity, it is *not* usually justified to write

$$\mathcal{G}=\sum_{p,q}\mid p\rangle\langle\tilde{p}\mid\mathcal{G}\mid q\rangle\langle\tilde{q}\mid. \tag{1}$$

This equation was presupposed in the derivations of *I* and *II*, so we must investigate whether this relation can be dispensed with. Before doing this, we note that $(H+\mathfrak{L})$ is not even Hermitian for some of the basis states used in the earlier derivations. The relation $(H+\mathfrak{L})^\dagger=H+\mathfrak{L}^*$ in matrix form

$$\langle\tilde{p}\mid H+\mathfrak{L}\mid q\rangle=\langle\tilde{q}\mid H+\mathfrak{L}\mid p\rangle \tag{7}$$

fails, in general, when $\mid p\rangle$ and $\langle q\mid$ contain unbound channel states, so Eq. (1) fails, since it involves *all* states $\mid p\rangle$ and $\langle q\mid$. The difference between the present (shell-model) basis and the others is that now Eq. (7) may fail even when $\mid p\rangle$ and $\mid q\rangle$ contain only bound shell-model channel states. In any case, Eq. (7) always fails for certain types of states p, q, so that Eq. (1) is incorrect. Thus, there is a flaw in I and II arising from the use of Eq. (1). We now show that the use of Eqs. (1) and (7) is unnecessary, and that a weaker Hermitian condition is sufficient to derive the reaction theories, including the "calculable" one.

The operator $(H+\mathfrak{L})$ is Hermitian with respect to two states ϕ and ψ, if and only if

$$\langle\tilde{\phi}\mid H+\mathfrak{L}\mid\psi\rangle-\langle\psi\mid H+\mathfrak{L}\mid\phi\rangle$$
$$=\int_I d\tau[\tilde{\phi}^*(H+\mathfrak{L})\psi-\tilde{\psi}^*(H+\mathfrak{L})\phi]=0, \tag{8}$$

where the integral is over the internal region I, and $\tilde{\phi}$ is the complex conjugate of time-reversed ϕ, as described in I. For certain kinds of ψ, ϕ, one may choose I such that the integral on terms in H can be transformed into a sum on two-body channel surfaces only. These terms are then cancelled off by the $\mathfrak{L}$ terms, so $(H+\mathfrak{L})$ is Hermitian. For other kinds, no choice of I will permit this, so that $(H+\mathfrak{L})$ is not Hermitian. The distinction between the two cases is according to whether at least one of ψ, ϕ has only two-body channel components or not. (When referring to channels, we always mean "actual" channels, i.e., those for the physical, not a model, system.) In Appendix B, we illustrate this condition by reference to the simple case of two particles in one dimension.

Thus, if ψ is the exact solution of H at an energy E, which is below the threshold fort hree-body break up (as is assumed in almost all resonance reaction theories), then $(H+\mathfrak{L})$ is Hermitian between ψ and model states $\mid p\rangle$, even when it is not Hermitian amongst the $\mid p\rangle$ themselves,

$$\langle\tilde{p}\mid H+\mathfrak{L}\mid\psi\rangle=\langle\tilde{\psi}\mid H+\mathfrak{L}\mid p\rangle,$$
$$\langle\tilde{p}\mid H+\mathfrak{L}\mid q\rangle\neq\langle\tilde{q}\mid H+\mathfrak{L}\mid p\rangle. \tag{9}$$

Consider now the expansion in I:

$$\mid\psi\rangle=\sum_q a_q\mid q\rangle, \tag{10}$$

where the $\mid q\rangle$ need not be orthogonal in I. On inserting this in the left-hand side of the Hermiticity property Eq. (9),

$$\sum_q\langle\tilde{p}\mid H+\mathfrak{L}-E\mid q\rangle a_q=\langle\tilde{p}\mid\mathfrak{L}\mid\psi\rangle \tag{11}$$

with the solution

$$\mid\psi\rangle=\sum_{p,q}\mid q\rangle(\mathbf{A}^{-1})_{qp}\langle\tilde{p}\mid\mathfrak{L}\mid\psi\rangle, \tag{12}$$

where we have defined $A\equiv H+\mathfrak{L}-E$. This result is now in a form which may be compared to the less general result

$$\mid\psi\rangle=\sum_{p,q}\mid q\rangle\langle\tilde{q}\mid A^{-1}\mid p\rangle\langle\tilde{p}\mid\mathfrak{L}\mid\psi\rangle, \tag{13}$$

which is valid when $\mid p\rangle$ is an orthogonal complete set with the property that $(H+\mathfrak{L})$ is Hermitian in the set.

From matrix algebra, if H is split into a zeroth-order

TABLE I. Classification of seven published theories of resonance reactions by $H-H^0$ and $\mathfrak{L}-\mathfrak{L}^0$.

Theory	$H-H^0$	$\mathfrak{L}-\mathfrak{L}^0$
Kapur-Peierls[a]	0	0
R-matrix (Wigner-Eisenbud)[b]	0	$\neq 0$
Brown-deDominicis[c]	0	0
Mandl, Kwok, and Herzenberg[d]	$\neq 0$	0
Feshbach[e]	$\neq 0$	0[f]
MacDonald[g]	$\neq 0$	0[f]
Analogue theory of II[h]	$\neq 0$	$\neq 0$

[a] Reference 12.
[b] Reference 13.
[c] Reference 18.
[d] Reference 25.
[e] Reference 15.
[f] Strictly, $\mathfrak{L}-\mathfrak{L}^0=0$ for closed channels. The choice for open channels is left open.
[g] Reference 14.
[h] Reference 2.

part H^0 and a residual interaction H'

$$H=H^0+H', \tag{14}$$

then

$$\mathbf{H}=\mathbf{H}^0+\mathbf{H}'$$

and

$$\begin{aligned}\mathbf{A}^{-1}&=(\mathbf{H}^0-\mathbf{E})^{-1}-\mathbf{A}^{-1}\mathbf{h}(\mathbf{H}^0-\mathbf{E})^{-1}\\&=(\mathbf{H}^0-\mathbf{E})^{-1}-(\mathbf{H}^0-\mathbf{E})^{-1}\mathbf{h}(\mathbf{H}^0-\mathbf{E})^{-1}\\&\quad+(\mathbf{H}^0-\mathbf{E})^{-1}\mathbf{h}\mathbf{A}^{-1}\mathbf{h}(\mathbf{H}^0-\mathbf{E})^{-1},\end{aligned} \tag{15}$$

where $\mathbf{h}$ is the matrix of $H'+\mathfrak{L}$. The wave function in Eq. (12) becomes

$$\begin{aligned}|\psi\rangle=&\sum_{p,q}|q\rangle[(\mathbf{H}^0-\mathbf{E})^{-1}]_{qp}\langle\tilde{p}\,|\,\mathfrak{L}\,|\,\psi\rangle\\&-\sum_{p,q,r,s}|q\rangle(\mathbf{A}^{-1})_{qp}\langle\tilde{p}\,|\,H'+\mathfrak{L}\,|\,r\rangle[(\mathbf{H}^0-\mathbf{E})^{-1}]_{rs}\\&\times\langle\tilde{s}\,|\,\mathfrak{L}\,|\,\psi\rangle.\end{aligned} \tag{16}$$

Special cases of Eqs. (15) and (16) for orthogonal states have recently been derived by Tobocman and Garside.[8]

In applications of Eqs. (15) and (16), the states $|\,p\rangle$ are eigenstates of H^0. Note that the set $|\,p\rangle$ may also be taken as eigenstates of $\mathfrak{L}$; $\mathfrak{L}\,|\,p\rangle=0$. This does not mean that the states $|\,p\rangle$ contain only channel components $|\,c\rangle$ on the surface of the interior region. For example, if $|\,p\rangle$ are shell-model states, then (if centroid motion is ignored) the relation $\mathfrak{L}\,|\,p\rangle=0$ is satisfied by choosing the single-particle wave functions to satisfy the outgoing wave condition.

Equations (12)–(16) are valid if $\mathfrak{L}$ is replaced by the more general $\mathfrak{L}(b)$. The expansions [Eqs. (12) and (13)] are the ones appropriate to the first two theories in Table I. For the other theories, a different set of expansion is needed. This depends on the use of an auxiliary function ϕ, which has the property that on the surface of I, it contains only those states of the residual nucleus which occur in the sum on c in $\mathfrak{L}$. Then, using the same method as for Eq. (12),

$$\begin{aligned}|\psi\rangle=|\phi\rangle+&\sum_{p,q}|q\rangle(\mathbf{A}^{-1})_{qp}\\&\times(\langle\tilde{p}\,|\,\mathfrak{L}\,|\,\psi-\phi\rangle-\langle\tilde{p}\,|\,H-E\,|\,\phi\rangle).\end{aligned} \tag{17}$$

If $\psi^{(c)}$ is the solution with incident flux only in channel c, and $\phi^{(c)}$ has the same property (with the same amplitude of incident flux), then

$$\mathfrak{L}\,|\,\psi^{(c)}-\phi^{(c)}\rangle=0$$

and

$$|\,\psi^{(c)}\rangle=|\,\phi^{(c)}\rangle-\sum_{p,q}|q\rangle(\mathbf{A}^{-1})_{qp}\langle\tilde{p}\,|\,H-E\,|\,\phi^{(c)}\rangle. \tag{18}$$

This equation leads to the other theories of Table I.

It is important to realize that Eq. (16) and Eq. (18) are not equivalent, even when ψ in Eq. (16) is specialized to $\psi^{(c)}$. They would clearly be the same if $\phi^{(c)}$ of Eq. (18) could be equated to

$$\sum_{p,q}|q\rangle[(\mathbf{H}^0-\mathbf{E})^{-1}]_{qp}\langle\tilde{p}\,|\,\mathfrak{L}\,|\,\psi^{(c)}\rangle \tag{19}$$

of Eq. (16). However this is not true, in general. The states $|\,q\rangle$ form a complete set, but the expansion of $\phi^{(c)}$ has this form only if $\phi^{(c)}$ is both an eigenstate of H^0, and if on the surface of I it contains only those residual states in the set $|\,c\rangle$ occurring in $\mathfrak{L}$. This can happen in certain model situations such as when the total system is a particle and a residual nucleus, which is simply a vibrator or a rotator, i.e., it has a limited number of excited collective (vibrational or rotational) states, all of them bound, and $H=H(\text{collective})+H(\text{particle})+H(\text{coupling})$. For actual nuclei, however, there is a real distinction between Eqs. (16) and (18). The fact that $\phi^{(c)}$ of Eq. (18) is restricted on the surface of I to contain only the states $|\,c\rangle$ occurring in $\mathfrak{L}$ means that it cannot be an eigenstate of an arbitrary H^0. Further, it is not an eigenstate of *any* H^0, except H itself. (It is not necessary to make $\phi^{(c)}$ antisymmetric, just because $\psi^{(c)}$ is, but it is usually very convenient to do so.)

In a related investigation,[17] it was found that $\mathbf{A}^{-1}$ could be ambiguous when taken in an over-complete infinite set of states $|\,p\rangle$, i.e., a set for which the unit operator $1=\sum_{p,q}|\,p\rangle U_{pq}\langle\,q\,|$ is nonunique in I. Thus, the above expansion of $|\,\psi\rangle$ may be unique only when the states $|\,p\rangle$ are orthogonal in I [this property is independent of the Hermiticity of $(H+\mathfrak{L})$]. For practical calculations, this is immaterial, since $\mathbf{A}^{-1}$ is taken in a truncated set and is then unique. Further, the possible nonuniqueness for an infinite set does not prejudice the use of the above formulas for $|\,\psi\rangle$ for

[17] A. M. Lane and D. Robson, Phys. Rev. **178**, 1715 (1969).

obtaining a reliable scattering matrix for a truncated set. We have already shown from other viewpoints[17] that the best form of the scattering matrix in terms of a truncated set corresponds to the expansion Eq. (12).

III. VARIOUS FORMS OF CALCULABLE THEORIES WITHOUT CONTINUUM STATES

Having derived the forms Eqs. (12), (16), and (18) for the wave function, it is straightforward to insert these in various expressions for the scattering or reactance matrices to get a variety of "calculable" theories.

A. Forms of the Scattering Matrix

1. *Kupur-Peierls Theory*

As shown in I, the Kapur-Peierls form[12] of the S matrix follows from inserting Eq. (13) in the expression:

$$S_{c'c}=i\hbar^{-1}(v_cv_{c'})^{-1/2}\langle\mathcal{O}_{c'}\mid\mathfrak{L}^*\mid\psi^{(c)}\rangle$$
$$=i\hbar^{-1}(v_cv_{c'})^{-1/2}(\langle\mathcal{O}_{c'}\mid\mathfrak{L}\mid\mathcal{I}_c\rangle+\langle\mathcal{O}_{c'}\mid\mathfrak{L}^*-\mathfrak{L}\mid\psi^{(c)}\rangle), \tag{20}$$

where v_c is relative channel velocity, $\mathcal{O}_c$, $\mathcal{I}_c$ are the total wave functions for outgoing, ingoing waves:

$$\mathcal{O}_c\equiv r_c^{-1}O_c(r_c)\mid c\rangle,$$
$$\mathcal{I}_c\equiv r_c^{-1}I_c(r_c)\mid c\rangle, \tag{21}$$

and $\psi^{(c)}$ is the exact solution with an ingoing wave in channel c only and so, in the external region,

$$\psi^{(c)}=\mathcal{I}_c-\sum_{c'}S_{cc'}(v_c/v_{c'})^{1/2}\mathcal{O}_{c'}. \tag{22}$$

On inserting Eq. (12) in Eq. (20), we get the Kapur-Peierls calculable formula

$$S_{c'c}=\frac{I_c(a_c)}{O_c(a_c)}\delta_{cc'}+i\frac{(2k_ca_c)^{1/2}}{O_c(a_c)}\frac{(2k_{c'}a_{c'})^{1/2}}{O_{c'}(a_{c'})}R_{c'c}, \tag{23}$$

where $k_c\equiv m_cv_c/\hbar$ and

$$R_{c'c}\equiv\sum_{p,q}\gamma_{pc'}(\mathbf{A}^{-1})_{pq}\gamma_{qc}, \tag{24}$$

$$\gamma_{qc}\equiv(\hbar^2a_c/2m_c)^{1/2}\langle r_c^{-2}\delta(r_c-a_c)c\mid q\rangle. \tag{25}$$

2. *Brown and deDominicis's Theory*

If $\phi^{(c)}$ are any set of functions with the property

$$\mathfrak{L}\phi^{(c)}=\mathfrak{L}\psi^{(c)}=\mathfrak{L}\mathcal{I}_c, \tag{26}$$

then it can be shown directly that the scattering matrix Eq. (20) may be rewritten as

$$i\hbar(v_cv_{c'})^{1/2}(S_{c'c}-S_{c'c}^0)=\langle\mathfrak{L}^*\tilde{\phi}^{(c')}\mid\psi^{(c)}-\phi^{(c)}\rangle, \tag{27}$$

where $S_{c'c}^0$ is defined as

$$i\hbar(v_cv_{c'})^{1/2}S_{c'c}^0\equiv-\langle\mathcal{O}_{c'}\mid\mathfrak{L}^*\mid\phi^{(c)}\rangle. \tag{28}$$

If $\phi^{(c')}$ further has the property that on the surface of I it contains only those states c occurring in $\mathfrak{L}$, then, using $(H-E)\psi^{(c)}=0$, we obtain

$$i\hbar(v_cv_{c'})^{1/2}(S_{c'c}-S_{c'c}^0)=-\langle\tilde{\phi}^{(c')}\mid H-E\mid\phi^{(c)}\rangle$$
$$-\langle(H-E)\tilde{\phi}^{(c')}\mid\psi^{(c)}-\phi^{(c)}\rangle. \tag{29}$$

Finally, insertion of solution Eq. (18) gives the Brown-deDominicis[18] calculable formula

$$i\hbar(v_cv_{c'})^{1/2}(S_{c'c}-S_{c'c}^0)=-\langle\tilde{\phi}^{(c')}\mid H-E\mid\phi^{(c)}\rangle$$
$$+\sum_{p,q}\langle(H-E)\tilde{\phi}^{(c')}\mid p\rangle(\mathbf{A}^{-1})_{pq}\langle\tilde{q}\mid(H-E)\mid\phi^{(c)}\rangle. \tag{30}$$

This may be compared with the formula obtained by inserting Eqs. (12) and (15) into Eq. (20):

$$i\hbar(v_cv_{c'})^{1/2}(S_{c'c}-\bar{S}_{c'c}^0)=-\langle\tilde{\chi}^{(c')}\mid H'+\mathfrak{L}\mid\chi^{(c)}\rangle$$
$$+\sum_{p,q}\langle\tilde{\chi}^{(c')}\mid H'+\mathfrak{L}\mid p\rangle(\mathbf{A}^{-1})_{pq}\langle\tilde{q}\mid H'+\mathfrak{L}\mid\chi^{(c)}\rangle, \tag{31}$$

where the functions $\chi^{(c)}$ are defined as

$$\mid\chi^{(c)}\rangle\equiv-(\hbar v_c)^{1/2}[(2k_ca_c)^{1/2}/O_c(a_c)]$$
$$\times\sum_{p,q}\mid p\rangle[(\mathbf{H}^0-\mathbf{E})^{-1}]_{pq}\gamma_{qc} \tag{32}$$

and

$$i\hbar(v_cv_{c'})^{1/2}\bar{S}_{c'c}^0\equiv-\langle\mathcal{O}_{c'}\mid\mathfrak{L}^*\mid\chi^{(c)}\rangle. \tag{33}$$

As remarked in the last section, the two results (30) and (31) are not the same when applied to actual nuclei, although they may be equivalent for certain simple models in which the target is represented as a vibrator or rotator, ignoring the fact that it is composed of particles like the incident one. Equation (30) expresses $S_{c'c}$ in terms of the auxiliary functions $\phi^{(c)}$, in addition to the set p, while Eq. (31) expresses $S_{c'c}$ entirely in terms of the set p [because of Eq. (32)].

Neither $S_{c'c}^0$ nor $\bar{S}_{c'c}^0$ is a true scattering matrix in general. $S_{c'c}^0$ will only be so if $\phi^{(c)}$ is the solution of a Hamiltonian. $\bar{S}_{c'c}^0$ is not the scattering matrix of H^0, because it involves actual channel states c, rather than the model channel states of H^0.

B. Forms for Reactance (R) Matrix

1. *Wigner-Eisenbud Theory*

The evaluation of the scattering matrix may be split into two stages, the first being the extraction of Wigner and Eisenbud's[13] R matrix. If $\mathbf{R}(b)$ is the R matrix for the real boundary conditions $b\equiv(b_c)$,

$$R_{c'c}(b)=\sum_{\lambda}[\gamma_{\lambda c'}\gamma_{\lambda c}/(E_\lambda-E)], \tag{34}$$

where $H\mid\lambda\rangle=E_\lambda\mid\lambda\rangle$, $\mathfrak{L}(b)\mid\lambda\rangle=0$, then $\mathbf{S}$ follows from

[18] G. E. Brown and C. T. deDominicis, Proc. Phys. Soc. (London) **A72**, 70 (1958).

Eq. (23) and

$$\mathbf{R}=(\mathbf{1}-\mathbf{R}(b)\mathbf{L})^{-1}\mathbf{R}(b), \tag{35}$$

where $\mathbf{L}$ is the diagonal matrix

$$L_{c'c}=\delta_{c'c}\{a_c[O_c'(a_c)/O_c(a_c)]-b_c\}. \tag{36}$$

To develop calculable forms for $\mathbf{R}(b)$, we may start from

$$R_{c'c}(b)=\langle\psi^{(c')}(b)|\,\mathfrak{L}(b)\,|\psi^{(c)}(b)\rangle$$
$$=\langle\mathfrak{L}(b)\psi^{(c')}(b)\,|\,\psi^{(c)}(b)\rangle. \tag{37}$$

This expresses $\mathbf{R}(b)$ in terms of exact solutions of $(H-E)\psi^{(c)}(b)=0$, where $\psi^{(c)}(b)$ satisfies the boundary conditions $b_{c'}$ in all channels c' except $c'=c$, where it is normalized by

$$\mathfrak{L}(b)\,|\,\psi^{(c)}\rangle=(\hbar^2a_c/2m_c)^{1/2}r_c^{-2}\delta(r_c-a_c)\,|\,c\rangle. \tag{38}$$

On using Eq. (12) applied to the case where $\mathfrak{L}$ is replaced by $\mathfrak{L}(b)$, the Wigner-Eisenbud calculable theory follows:

$$R_{c'c}(b)=\sum_{p,q}\gamma_{pc'}(\mathbf{A}^{-1}(b))_{pq}\gamma_{qc}. \tag{39}$$

2. *R-Matrix Versions of Brown-deDominicis Theory*

The essential feature of Brown-deDominicis theory is that matrix elements $\langle\tilde{q}\,|\,H-E\,|\,\phi^{(c)}\rangle$ occur in the theory rather than surface amplitudes γ_{qc}. To obtain the R matrix of such a theory, we may start from Eq. (37) and develop it into

$$R_{c'c}(b)-R_{c'c}{}^0(b)=\langle\mathfrak{L}(b)\phi^{(c')}(b)\,|\,\psi^{(c)}(b)-\phi^{(c)}(b)\rangle$$
$$=-\langle\phi^{(c')}(b)|(H-E)|\,\phi^{(c)}(b)\rangle$$
$$-\langle(H-E)\phi^{(c')}(b)\,|\,\psi^{(c)}(b)-\phi^{(c)}(b)\rangle, \tag{40}$$

where $R_{c'c}{}^0(b)$ is defined as

$$R_{c'c}{}^0(b)=\langle\mathfrak{L}(b)\phi^{(c')}(b)\,|\,\phi^{(c)}(b)\rangle \tag{41}$$

and the $\phi^{(c)}(b)$ are any set of functions which contain only states c on the surface of I and satisfy the same boundary condition Eq. (38) as $\psi^{(c)}(b)$. Insertion of Eq. (18) gives the required result:

$$R_{c'c}(b)-R_{c'c}{}^0(b)=-\langle\phi^{(c')}(b)|\,H-E\,|\,\phi^{(c)}(b)\rangle$$
$$+\sum_{p,q}\langle(H-E)\phi^{(c')}(b)|\,p\rangle(\mathbf{A}^{-1}(b))_{pq}\langle\tilde{q}\,|\,H-E\,|\,\phi^{(c)}(b)\rangle. \tag{42}$$

These results apply when $\phi^{(c)}(b)$ is intrinsically complex (as when it is the solution of a complex potential) provided that $\langle\phi^{(c')}(b)|$ is replaced everywhere by $\langle\tilde{\phi}^{(c')}(b)|$.

The result [Eq. (42)] may be compared to that obtained by the insertion of Eq. (15) in Eq. (39) [with $\mathfrak{L}(b)$ instead of $\mathfrak{L}$]

$$R_{c'c}(b)-\bar{R}_{c'c}{}^0(b)=-\langle\chi^{(c')}(b)|\,H'+\mathfrak{L}(b)\,|\,\chi^{(c)}(b)\rangle$$
$$+\sum_{p,q}\langle\chi^{(c')}(b)|\,H'+\mathfrak{L}(b)\,|\,p\rangle(\mathbf{A}(b)^{-1})_{pq}$$
$$\times\langle\tilde{q}\,|\,H'+\mathfrak{L}(b)\,|\,\chi^{(c)}(b)\rangle, \tag{43}$$

where $\bar{R}_{c'c}{}^0(b)$ is defined as

$$\bar{R}_{c'c}{}^0(b)\equiv\langle\mathfrak{L}(b)\chi^{(c')}(b)\,|\,\chi^{(c)}(b)\rangle, \tag{44}$$

and the functions $\chi^{(c)}(b)$ are defined as

$$|\,\chi^{(c)}(b)\rangle=\sum_{p,q}|\,p\rangle[(\mathbf{H}^0-\mathbf{E})^{-1}]_{pq}\gamma_{qc}. \tag{45}$$

The comments made below Eq. (33) apply here. Equations (42) and (43) are not the same expressions, in general. They are the same when applied to certain model systems, but not when applied to actual nuclei.

Equation (43) has been derived by Tobocman and Garside[8] in the special case when the states $|\,p\rangle$ are orthogonal states satisfying $\mathfrak{L}(b)\,|\,p\rangle=0$.

IV. COMPARISON OF NUMERICAL ACCURACY AND CALCULATIONAL PROPERTIES OF VARIOUS FORMS

Buttle[19] has made a study of two of the calculable forms of Sec. III in the special circumstances of a particle-plus-rotator system, where the latter has just two states. This system can be solved exactly, and the accuracy of the various forms can be compared. The following is a summary of the properties of the various forms.

A. Wigner-Eisenbud Theory Eq. (39)

As Buttle[19] pointed out, one cannot expect to get accurate results by simply truncating the orthogonal set of states p, q in Eq. (39), and retaining only those states occurring near the energy region of interest. The reason is that when orthogonal states are used, distant terms have values of γ_{pc} as large as nearby ones, and also their relative importance declines only as the first inverse power of energy. Thus, distant terms must be retained, even though it is not practical to include them in the actual inversion of $\mathbf{A}$. In the special case when the states p are orthogonal states of a model Hamiltonian H^0, which has the same channel states as H, the appropriate approximate form of $\mathbf{R}$ is[19]

$$R_{c'c}(b)=R_{c'c}(b,H^0)-\sum_p{}'[\gamma_{pc'}\gamma_{pc}/(E_p-E)]$$
$$+\sum_{p,q}{}'\gamma_{pc'}(\mathbf{A}(b)^{-1})_{pq}\gamma_{qc}, \tag{46}$$

where the prime denotes that all states p, q are restricted

[19] P. J. A. Buttle, Phys. Rev. **160**, 719 (1967).

to the truncated set, and $R_{c'c}(b, H^0)$ is the R matrix of H^0

$$R_{c'c}(b, H^0) \equiv \sum_p [\gamma_{pc'}\gamma_{pc}/(E_p - E)]. \quad (47)$$

A rationale for Eq. (46) may be obtained from giant-resonance theory,[20] viz., any given state p is coupled strongly only to states q within a certain energy range (provided H^0 is chosen to best advantage). Thus, while we must treat the mixing within nearby levels properly, that between "nearby" and "distant" and between "distant" and "distant" levels may be ignored.

When the states p are not orthogonal, the appropriate procedure is less evident, because states may no longer be termed "nearby" or "distant" in unambiguous fashion. Some formal developments of Eq. (39) for nonorthogonal states are made in Appendix C. Recently calculations have been carried out by Adams[21] and Purcell[22] using nonorthogonal states according to the methods discussed in Ref. 1. In contrast to the more conventional orthogonal state calculations, the nonorthogonal calculations do not require the inclusion of any contributions from distant states. It was found that the use of nonorthogonal states leads to a very rapid convergence rate as the number of states included is increased. This is an important simplification, since it means that only the last term in Eq. (46) needs to be calculated when $|p\rangle$, $|q\rangle$ are the appropriate nonorthogonal states.

The essential calculational needs of the Wigner-Eisenbud method are

(1) a single diagonalization of the real level matrix of $(H+\mathfrak{L}-E)$, *or* the inversion for a series of energies of the real matrix of $(H+\mathfrak{L}-E)$,

(2) an inversion of the complex channel matrix $\mathbf{1}-\mathbf{R}(b)\mathbf{L}$ in Eq. (35), in order to obtain S from Eqs. (23) and (35). This inversion must be done at each of a sequence of energies through the energy range of interest.

B. Kapur-Peierls Theory Eq. (24)

This was not used by Buttle. The above comments preceding Eqs. (46) and (47), and the equations themselves apply here. However, the calculational needs are different, since the present theory contains the operator $\mathfrak{L}$, which is complex and energy-dependent [unlike $\mathfrak{L}(b)$ which is real and energy-independent if the b_c are]. The needs are the inversion of the complex level matrix of $(H+\mathfrak{L}-E)$ at each of a sequence of energies through the region of interest.

C. Brown-deDominicis Theory Eq. (30)

This form has the merit over the conventional Wigner-Eisenbud method in that distant levels are included systematically by the presence of $S_{c'c}^0$. The set used in the last term of Eq. (30) may be truncated without introducing any new term to account for distant levels, provided that the auxiliary functions $\phi^{(c)}$ (which define $S_{c'c}^0$) are chosen properly.

The calculational need of this method is the inversion of a series of energies of the complex level matrix of $(H+\mathfrak{L}-E)$.

The disadvantages of this method relative to the Wigner-Eisenbud one are

(1) it cannot be treated as a single diagonalization of a level matrix. (This is significant only if the number of channels is smaller than the number of levels, since the Wigner-Eisenbud theory involves the inversion of a channel matrix.)

(2) The approximation caused by the truncation means that the theory is nonunitary (whereas the Wigner-Eisenbud theory is always unitary).

(3) In the computational area, Buttle[19] found that small spurious peaks can arise from Eq. (24). In principle, the terms on the right generate the observed resonances and replace the original auxiliary resonances from $S_{c'c}^0$ by these. In practice, the resonances of $S_{c'c}^0$ are not fully cancelled out, so that spurious resonances remain.

In the model used by Buttle, Eqs. (30) and (31) are the same, so there is no evidence on the relative merits of the two forms.

D. R-Matrix Version of Brown and deDominicis Theory [Eq. (42)]

This again has the merit over the conventional Wigner-Eisenbud method Eq. (39) that distant level effects are built into the method. For $\phi^{(c)}$ real, this method involves only real quantities, and is thus always unitary. For complex $\phi^{(c)}$, complex quantities occur and, after truncation unitarity is not ensured. Its computational needs are the same as those of the Wigner-Eisenbud method cited above.

This form was not examined by Buttle, and there remains an important question over the practical merit of this hybrid method: Will it suffer the snag of the Brown-deDominicis method that the original resonances in $R_{c'c}^0$ are not fully cancelled out, so that spurious resonance effects occur?

V. PRACTICAL USE OF CALCULABLE THEORIES WITH SHELL-MODEL WAVE FUNCTIONS

When shell-model states are used for the truncated set $|p\rangle$ in the calculable forms of Sec. III, we obtain theories which may be described as the counterparts of the Bloch-Fano theory corresponding to a finite interior region. Here we will comment on a number of points, both formal and practical, that are met in using shell-model states.

[20] A. M. Lane, R. G. Thomas, and E. P. Wigner, Phys. Rev. **98**, 693 (1955).

[21] J. L. Adams, Ph.D. thesis, Florida State University, 1967 (unpublished).

[22] J. E. Purcell, Phys. Rev. **185**, 1278 (1969).

A. Completeness

Ignoring such complications as centroid motion and composite particles (see below), we may assert that, if the shell-model radius R is large enough, then the channel surfaces of the interior region I may be said to lie on (or inside) the shell-model surfaces S_i defined by $|\mathbf{r}_i|=R$; $|\mathbf{r}_j|<R$. It then follows that the shell-model states $|p\rangle$ constitute a complete set in I. An apparent difficulty arises from the fact that the surface integrations occurring in the theories of Sec. III are over all values of the internal coordinates from zero to infinity, while the shell-model surface S_i allows integration up to R only. This will not be important however, since the integrand always contains the internal wave functions of the target states and I is defined such that these must be very small at distances $\geq R$ (otherwise, three-body channel surfaces would be necessary).

B. Sources of Error

The formulas of Sec. III are exact provided that:

(a) The set of states $|p\rangle$ is complete.

(b) $(H+\mathfrak{L})$ is Hermitian between ψ and p, which will be so if

(1) The wave functions of the residual nuclei (essentially $|c\rangle$) should be consistent with the Hamiltonian H, i.e., they should be the correct channel solutions of H. Further $\mathfrak{L}$ must include all open channels $|c\rangle$.

(2) The radius a is large enough to make all $|c\rangle$ negligibly small when one of the constituent particles in the residual nucleus is at or outside this radius. [Of course, this condition could not be satisfied if any unbound residual nuclei occurred in the channel states $|c\rangle$. This is why it is always assumed that the energy is below the three-body break-up threshold (see Appendix B).] This condition means that it is immaterial whether the internal coordinate integrations occurring in the evaluation of γ_{pc} are taken over all space or only inside radius a.

In practical calculations, all three conditions (a), (1), and (2) are violated to some extent. One must be careful that the corresponding errors in the scattering matrix are not amplified. For example, because of violation of (a), uncritical use of the Wigner-Eisenbud or Kapur-Peierls methods, Eq. (24) or Eq. (39), can lead to large error, even when many states are included. As we have seen in Sec. IV in the case of orthogonal representations, this error arises from distant states, and can be eliminated by including them in their zeroth-order form, i.e., without any diagonalization of $(H+\mathfrak{L})$. The final error should be no larger than the minimal error due to truncation, i.e., of relative order $[\langle\psi|\psi\rangle-\sum_p\langle\psi|p\rangle^2]/\langle\psi|\psi\rangle$. Of course this will not be true if the choice of $|p\rangle$ is perverse, e.g., if $\gamma_{pc}\approx 0$ for all p. Then the scattering matrix element S_{cc} will have large error.

For actual nuclei, with two-body forces in H, condition (1) implies that states of residual nuclei in $|c\rangle$ should have two-particle correlations in them. Thus, the common approximation of using pure configuration states for these nuclei not only introduces error *per se*, but also because it is inconsistent with the form of H used in the evaluation of $\mathbf{A}^{-1}$. However, there is no reason to suspect that this latter error is larger than the former. Another aspect of condition (1) is that all open channels should be included. In the commonly used example of $N^{15}+p$, for energies up to 10 MeV, this means that all excited states of N^{15} below 10 MeV, not just the $1p_{3/2}^{-1}$ state, should be included.

Condition (2) can be satisfied, once the states of the residual nuclei are specified, by choosing the channel radii to be large enough. A consequence of (2) is that the exact solution ψ has a unique expansion on the surface of I in terms of states $|c\rangle$. The condition has been discussed in this form of a "channel orthogonality condition" by Danos and Greiner,[11] and recently by Mahaux and Weidenmuller.[23]

C. Character of States p

Bound-state shell-model calculations normally use either a finite well (like the Saxon-Woods one) or an infinite well (like the oscillator). Given the choice, the latter is usually used because of the simple analytical nature of the solutions. However, it cannot be used in reaction theories with no internal region, since its wave functions all vanish at infinity, i.e., there is no continuum. When an internal region is distinguished, as in the theories of Sec. III, there is no problem with infinite wells. They provide discrete sets of states p which are complete in the internal region, just as finite wells do. In fact, the formal distinction between the two kinds of well is of little relevance for the theories of Sec. III. Both can provide a set of discrete particle states from which the shell-model wave functions are constructed. The usual oscillator functions which vanish at infinity can be used. The fact that the higher orbitals are not orthogonal to each other inside the radius a of I does not matter, since the orthogonality of states $|p\rangle$ is not assumed in Sec. III. If a finite well is used, then a discrete complete set of states can be set up by a boundary condition at the radius a or outside it.

D. Character of Channel States c

If the residual states c are approximated by pure configurations, then the channel orthogonality condition (2) is satisfied if the radius $r=a$ of I is taken outside the range of orbits that are occupied in the states c. However, a certain conflict is met in calculations which

[23] C. Mahaux and H. A. Weidenmüller, Phys. Rev. **170**, 847 (1968).

go beyond the use of pure configurations, and include correlations by allowing admixtures from a restricted number of unoccupied states. Such admixtures may represent correlations rather well in the body of the nucleus, but will not do so at the surface. In fact, since the unoccupied orbitals can be large at $r=a$, they can lead to a nonzero value of the residual state at $r=a$, and to a violation of (2). If all configuration mixing were included, in such a way that the correct binding energy was maintained, then this would be cancelled off by the higher states. Thus, if one seeks to go beyond the use of pure configurations for residual states, one must be careful that any spurious surface effects arising from violation of (2) do not offset the improvement one could normally expect. This problem of spurious effects cannot be solved simply by choosing the radius a to be larger. For finite wells, this will not reduce the size of positive energy orbitals at $r=a$. For infinite wells, all orbitals in c will be reduced, but so will the orbitals of the residual nucleon in many of the states p, so that the γ_{pc} become very small, and far more higher states p must be included to get sensible results.

The problem with residual states c of including configuration mixing from higher orbitals may be regarded as the counterpart in the present approach of the problem encountered by Bloch and Fano, viz., that they could not formulate a theory when the residual states included any continuum components. In the latter theory, the problem is one of principle, while in the present approach it is confined to the calculational area. Since the *actual* states c satisfy the condition (2) for a suitably chosen radius, one can assert that the approximate forms will also satisfy (2) if sufficient configuration mixing is properly included. There is a problem only when the mixing is restricted so that spurious surface effects in states c are not cancelled out.

Finally, it may be noted that the problem of spurious surface effects is probably more serious for the Wigner-Eisenbud and Kapur-Peierls theories, where the surface amplitudes γ_{pc} are directly affected by spurious effects. Thus one may expect that the effects will be reduced by using the Brown-deDominicis forms involving matrix elements $\langle \tilde{p} \mid H-E \mid \phi^{(c)} \rangle$. However, as remarked in Sec. IV, these forms have the disadvantage that spurious resonances may be generated when the set p is truncated severely, so that one cannot say at this stage if there is any net advantage. This is an important question, requiring further study.

E. Centroid Motion

The fact that shell-model wave functions do not have a fixed centroid causes no difficulty as far as completeness goes. I may still be said to be contained in the shell-model internal region, $\mid \mathbf{r}_i \mid \leq R$ for all i. The latter region has three more coordinates than I, which is defined in the space of relative coordinates only. Thus, if R is chosen large enough, the latter region contains I, and the states $\mid p \rangle$ form a complete set for the expansion of the exact wave function ψ with fixed centroid

$$\psi(\xi) = \sum_{\rho} a_p \psi_p(\xi, \varrho), \qquad (\text{all } \varrho)$$

where ϱ is the centroid coordinates and ξ are internal coordinates. When the sum in truncated, the resulting approximate ψ depends on ϱ to some extent. Generally, one may expect the best expansion with $\varrho=0$, since this is the mean value of the centroid position in ψ_p, although the rms value $\neq 0$. As the mass A of the system increases, the rms values of $\mid \varrho \mid$ decrease as $1/A$, at least, for low excitations. In the limit $\psi_p(\xi, \varrho) \rightarrow \chi_p(\xi)\delta(\varrho)$. Thus, for many particles, one expects the redundancy of coordinates in the shell-model states to have a small $1/A$ effect. For small numbers, the effects may be more serious, since the approximate ψ will not fall off sharply with increasing $\mid \varrho \mid$, but remains large and varies considerably.

F. Composite Particle Channels

Nothing has been said so far of the possibility of two-body channels for composites like deuterons. These give rise to no formal difficulties since, as with centroid motion, we may consistently assume that the shell-model region contains I, even when the latter has surfaces for composites. The only difference is that the surface of I can no longer be said to lie in the shell-model surface since the surface for a composite cuts across the shell-model surfaces. (For example, the deuteron surface for particles i, j is essentially $\mid \mathbf{r}_i + \mathbf{r}_j \mid$ = const, and this cuts $\mid \mathbf{r}_i \mid$ = const, $\mid \mathbf{r}_j \mid$ = const.) This introduces the complication that states $\mid p \rangle$ are not orthogonal in I, but this is a calculational, not a formal, problem.

VI. CONCLUSIONS

The advantages and disadvantages of the present kind of calculable shell-model theory relative to the original Fano-Bloch version are evident. On the credit side, the distinction between bound and continuum states is eliminated. In the original theory,[4,5] this division is very deep. The four parts of the interaction arising from this division (continuum-continuum, continuum-bound, etc.) appear in different ways in the results, despite the fact that they all stem from the same interactions between the same particles, and these interactions are exactly the same whether the particles are bound or free. Further, in practical calculation, the division is increased since the continuum-continuum interaction raises problems of its own which require special developments.[6,7] Another merit is that no restriction is imposed on the structure of target states; antisymmetrization (which causes a restriction in the original theory) does not cause any difficulties.

On the debit side, a division is made between the interior and exterior regions of space, which does not occur in the original theory. While possibly not beautiful, it is not clear that this division is any more artificial than the above division between bound and continuum states. Physically one can find arguments on both sides. An obvious instance is the presence of a narrow single-particle resonance. In the original theory, unless special provision is made, such resonances are part of the continuum, and are not explicitly introduced with the consequence that there are sharp energy variations in the interaction matrix elements. In the new version, such resonances appear on the same footing as others. On the other hand, the Fano-Bloch theory handles the distant, broad, single-particle levels in a more natural way. They are never separated out, and their effects appear in the form of a potential scattering phase shift and wave function. This is also true of the Brown-deDominicis formulas of Sec. III, but the conventional Kapur-Peierls and Wigner-Eisenbud formulas involve the explicit display of distant levels. However the appropriate nonorthogonal representation of the latter theories[17,21,22] appears to remove this problem. For the specific purposes of ease of calculation and achievement of accuracy, we believe that the present approach has distinct advantages. It avoids the use of continua, and the consequent calculational complications; antisymmetry is no problem; the calculation for an entire energy range can be reduced to the single diagonalization of an energy level matrix, plus the inversion of a channel matrix at a series of energies in the range. The most serious problem is that discussed under D of Sec. V: viz., that of maintaining the channel orthogonality condition (2) in calculations where configuration mixing effects are included in the residual states c.

APPENDIX A: DERIVATION OF THE BLOCH-FANO THEORY IN COMPREHENSIVE FORMALISM

The Bloch-Fano results may be obtained just like the Rodberg-MacDonald[14,24] ones of I by exchanging the roles of the discrete and continuum states. Equations (86) and (88) of I give

$$i\hbar(v_c v_{c'})^{1/2}[S_{c'c}-S_{c'c}(H_0)]=-\langle\tilde{\phi}^{(c')}\mid P_c\hat{S}P_c\mid\phi^{(c)}\rangle, \tag{A1}$$

where $S_{c'c}(H_0)$ is the scattering matrix for the shell-model Hamiltonian H_0, $\phi^{(c)}$ is the solution of H_0 with incoming waves in channel c, P_c projects on continuum states, and

$$\hat{S}=\Delta-\Delta\mathcal{G}\Delta, \tag{A2}$$

where

$$\Delta\equiv H-H_0. \tag{A3}$$

MacDonald and Rodberg develop S so as to display discrete states d as intermediate states. Equation (90) of I is

$$\hat{S}=\hat{y}-\hat{y}P_d[P_d(H+\mathfrak{L})P_d-E+P_d\hat{y}P_d]^{-1}P_d\hat{y}, \tag{A4}$$

where P_d projects on discrete states, $P_c+P_d=1$, and

$$\hat{y}=\Delta-\Delta P_c[P_c(H+\mathfrak{L})P_c-E]^{-1}\Delta. \tag{A5}$$

Using the notation of Bloch, e.g.,

$$\Delta^{cc}\equiv P_c\Delta P_c, \tag{A6}$$

$$\Delta_{(c)}{}^{cd}=\Delta^{cd}-\Delta^{cc}[P_c(H+\mathfrak{L})P_c-E]^{-1}\Delta^{cd}, \tag{A7}$$

then Eq. (A4) leads to

$$P_c\hat{S}P_c=\Delta_{(c)}{}^{cc}-\Delta_{(c)}{}^{cd}(H+\mathfrak{L}-E+\Delta_{(c)}{}^{dd})^{-1}\Delta_{(c)}{}^{dc}. \tag{A8}$$

In an exactly similar way, one may derive an alternative expression in which states d are eliminated instead of states c

$$P_c\hat{S}P_c=\Delta_{(d)}{}^{cc}-\Delta_{(d)}{}^{cc}(H+\mathfrak{L}-E+\Delta_{(d)}{}^{cc})^{-1}\Delta_{(d)}{}^{cc}. \tag{A9}$$

Inserting Eq. (A9) into Eq. (A1) gives the Bloch-Fano theory when the radii in $\mathfrak{L}$ are taken to ∞ so that[16] $\mathfrak{L}\longrightarrow -i\epsilon$.

APPENDIX B: SIMPLE MODEL TO ILLUSTRATE HERMITICITY CHARACTERISTICS OF REACTION SITUATIONS

Consider two particles in one dimension with positions x_1, x_2. Suppose that each particle feels a fixed potential centered at the origin in the interval $(-\alpha, +\alpha)$, and that this potential has bound states. Suppose that the interaction between particles has a bound state ("deuteron") with smaller binding than the lowest bound states of the potential.

Green's theorem gives

$$\int_v d\tau(\phi H\psi-\psi H\phi)=\frac{\hbar^2}{2m}\int_S d\sigma\left(\psi\frac{\partial\phi}{\partial n}-\phi\frac{\partial\psi}{\partial n}\right), \tag{B1}$$

where the left-hand integral is over any area v in the (x_1x_2) plane, and the right-hand one is over the boundary S of the area, $\partial/\partial n$ denotes differentiation normal to S. ψ will be taken to be an actual scattering state for energy E while ϕ is any arbitrary function.

The problem of interest is to see under what conditions the integral on S can be written as a sum over channels, thereby permitting the introduction of an $\mathfrak{L}$ operator such that $(H+\mathfrak{L})$ is Hermitian.

Elastic Scattering

First, suppose that the energy is below the threshold for deuteron production, and that there is only one bound state, viz., $u_b(x)$. This means that for x_1 large, the only nonzero part of ψ in the (x_1, x_2) plane has the product form $u_b(x_2)u_E(x_1)$, and is a strip along the x_1

[24] L. Rodberg, Phys. Rev. **124**, 210 (1961).

axis of constant width $2L_0$ (say), where this is essentially the size of the bound state. $u_E(x)$ is the scattering state of the potential. We may set up channel surfaces at the points where the strip begins to broaden out when x_1 is reduced (see Fig. 1). Below these points, ψ ceases to have product form because the particles interact. If the range of interaction is μ, the surfaces are $x_1 = \pm(L_0+\mu)$. Similar surfaces occur at $x_2=\pm(L_0+\mu)$. On drawing S through these four surfaces, the above surface term becomes

$$-\frac{\hbar^2}{2m}\left(u_E'(L_0+\mu)\int_{-L_0}^{+L_0} dx_2 u_b(x_2)\phi - u_E(L_0+\mu)\int_{-L_0}^{+L_0} dx_2 u_b(x_2)\frac{d\phi}{dx_1}\right) \quad \text{(B2)}$$

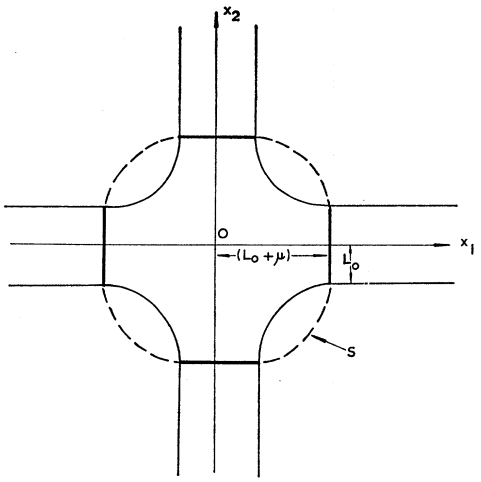

FIG. 1. Interior region and channels. The solid lines enclose the region where ψ is not negligibly small. The four heavy lines are the channel surfaces.

plus similar terms with $x_1 \leftrightarrow x_2$. The four connecting pieces of S contribute nothing since ψ vanishes on them.

Deuteron Production

As the energy approaches the deuteron threshold from below, the region of nonzero ψ begins to extend along the diagonal $x_1=x_2$ [Fig. 2(a)]. However, by drawing around the extensions, the surface integral still contains only the four channel-surface contributions. When the threshold is passed, the extension reaches to infinity, and it is not possible to connect the four surfaces without crossing them. Thus two new channel surfaces for deuterons must be drawn. If these are such that ψ has product form, they will be separated from the previous surfaces by regions of null ψ [Fig. 2(b)]. Thus, the surface integral now has the form of a sum over six channel surfaces.

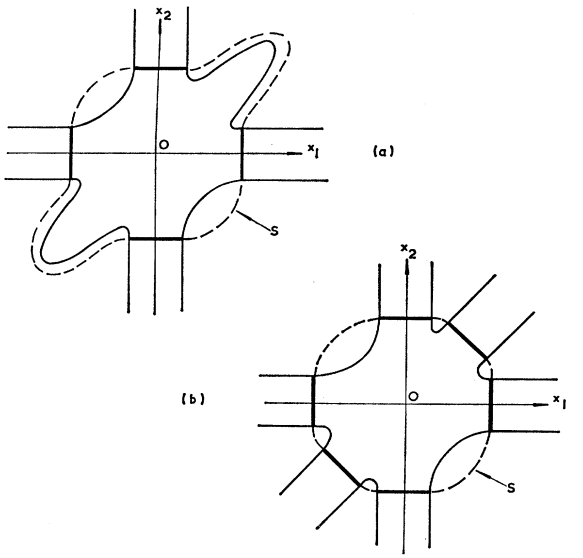

FIG. 2. In (a) the energy is below the deuteron threshold while in (b) it is above. In (a), S can be drawn to contain nucleon surfaces only, but in (b) it must include deuteron surfaces also.

Inelastic Scattering

When there is a second bound state, and the energy approaches the threshold from below, the region of nonzero ψ begins to spread along the axes in a band of width $2L_1$ rather wider than $2L_0$ (since an excited state has a larger spread). S will continue to have only the original four surface parts if these surfaces are redrawn beyond the new nonnull regions [Fig. 3(a)]. This is no longer

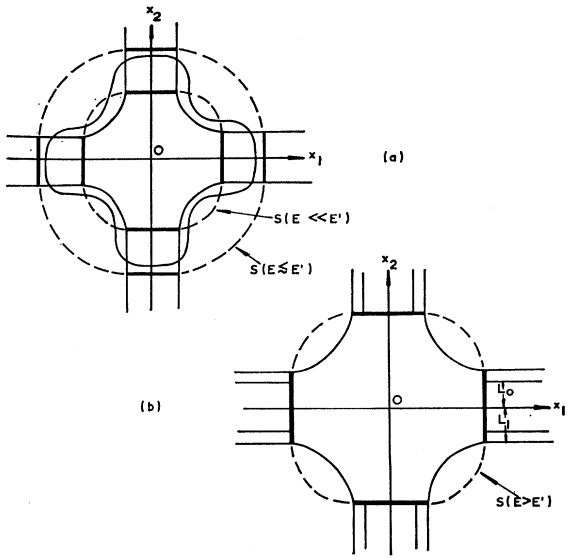

FIG. 3. In (a) the energy is below the threshold E' for inelastic scattering, while in (b) it is above. In (a) the inner and outer solid lines enclose the regions of non-negligible ψ arising from the ground and excited target states, respectively, when E is just less than E'.

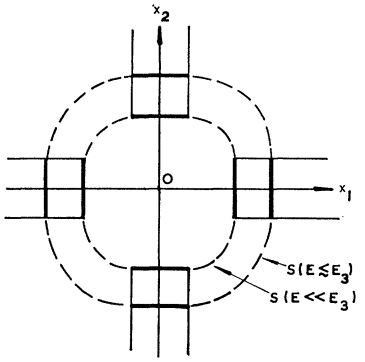

FIG. 4. The extension of the region of nonzero ψ as the energy E approaches the three-body break-up threshold E_3. The inner region expands into the outer region as E increases, and S must be correspondingly increased. Deuteron channels are suppressed for clarity.

possible when the threshold is crossed. In that case, if the surfaces are drawn at $x_1=\pm(L_1+\mu)$, $x_2=\pm(L_1+\mu)$ [Fig. 3(b)], each of the four surface integrals contains two terms corresponding to the fact that outside S the function ψ has the form (e.g., for $|x_1|\geq L_1+\mu$)

$$\psi=u_{b_0}(x_2)u_E^{(0)}(x_1)+u_{b_1}(x_2)u_E^{(1)}(x_1). \quad \text{(B3)}$$

This form is unique, since the u_b are orthogonal and the coefficients are given by

$$u_E^{(i)}(x_1)=\int_{-L_i}^{+L_i}\psi(x_1,x_2)u_{b_i}(x_2)dx_2 \quad \text{(B4)}$$

for $|x_1|\geq L+\mu$. Thus, each inelastic channel contributes its own channel-surface integral. Channel surfaces could be taken at different points for different inelastic channels without any contradiction arising.

In summary, we see that, for all open two-body channels, $(H+\mathfrak{L})$ is Hermitian, where

$$\mathfrak{L}=\sum_c|c\rangle\frac{\hbar^2}{2m_c}\delta(L_c+\mu-x_c)\left(\frac{d}{dx_c}-b_c\right)\langle c| \quad \text{(B5)}$$

and $|c\rangle$ are the channel states (i.e., the internal wave functions).

Three-Body Channels

As the energy approaches the threshold for two free nucleons (corresponding to three-body break up), the region of nonzero ψ grows radially outwards, forcing a larger and larger choice of S (Fig. 4). If S is not increased, then at $x_1=(L+\mu)$, the function ψ will contain significant amounts of unbound states $\mu_\epsilon(x_2)$. Since these extend over all x_2, while the surface integral is restricted to $|x_2|<L$, the orthogonality of u_b and u_ϵ does not operate to make the expansion of ψ unique.

There is no natural definition of finite channel surfaces for three-body processes. Thus when the energy passes the threshold, ψ is nonzero everywhere, and no construction of S is possible. It follows that the surface integral cannot be expressed as a channel sum, and there exists no channel-sum form of $\mathfrak{L}$ such that $(H+\mathfrak{L})$ is Hermitian.

APPENDIX C: NONORTHOGONAL STATES AND SEPARATION OF "NEARBY" AND "DISTANT" STATES

In the standard theories[12–15,18,25] of resonance phenomena, the states used as a basis for the resonances are assumed to be orthogonal, either over all space or over a restricted region. In the situation encountered in the more general theory, one may have a nonorthogonal basis. In this event, the separation of the collision matrix into nearby and "distant" levels becomes a nontrivial exercise.

The appropriate unit operator takes the form[17] (wherein M is the subspace of "nearby" levels p, q, and r is that of all other levels l, k)

$$1=\sum_{p,q=1}^{M}|p\rangle N_{pq}\langle\tilde{q}|+\sum_{l,k=M+1}^{\infty}|l\rangle X_{lk}\langle\tilde{k}| \quad \text{(C1)}$$

and the most general Green's operator may be written

$$\begin{aligned}\mathcal{G}(b)\equiv&[H+\mathfrak{L}(b)-E]^{-1}\\ =&\sum_{p,q}|p\rangle(\mathbf{G}_{MM})_{pq}\langle\tilde{q}|+\sum_{p,l}|p\rangle(\mathbf{G}_{Mr})_{pl}\langle\tilde{l}|\\ &+\sum_{k,q}|k\rangle(\mathbf{G}_{rM})_{kq}\langle\tilde{q}|+\sum_{k,l}|k\rangle(\mathbf{G}_{rr})_{kl}\langle\tilde{l}|,\end{aligned}$$

wherein

$$(\mathbf{G}_{Mr})_{pl}\equiv\sum_{q,k}N_{pq}(\mathcal{G}(b))_{qk}X_{kl}$$

and three similar equations are involved for $\mathbf{G}_{MM}$, $\mathbf{G}_{rr}$, and $\mathbf{G}_{rM}$. Defining $A\equiv H+\mathfrak{L}(b)-E$ and using $\mathcal{G}(b)A=1$, we obtain the matrix equations

$$\begin{pmatrix}\mathbf{G}_{MM}&\mathbf{G}_{Mr}\\ \mathbf{G}_{rM}&\mathbf{G}_{rr}\end{pmatrix}\begin{pmatrix}\mathbf{A}_{MM}&\mathbf{A}_{Mr}\\ \mathbf{A}_{rM}&\mathbf{A}_{rr}\end{pmatrix}=\begin{pmatrix}1&0\\ 0&\mathbf{X}\end{pmatrix}, \quad \text{(C2)}$$

which have the solutions

$$\begin{aligned}\mathbf{G}_{MM}&=(\mathbf{A}_{MM}-\mathbf{A}_{Mr}\mathbf{A}_{rr}^{-1}\mathbf{A}_{rM})^{-1},\\ \mathbf{G}_{Mr}&=-\mathbf{G}_{MM}\mathbf{A}_{Mr}\mathbf{A}_{rr}^{-1},\\ \mathbf{G}_{rM}&=-\mathbf{A}_{rr}^{-1}\mathbf{A}_{rM}\mathbf{G}_{MM}, \quad \text{(C3)}\\ \mathbf{G}_{rr}&=\mathbf{X}\mathbf{A}_{rr}^{-1}+\mathbf{A}_{rr}^{-1}\mathbf{A}_{rM}\mathbf{G}_{MM}\mathbf{A}_{Mr}\mathbf{A}_{rr}^{-1},\end{aligned}$$

[25] A. Herzenberg, K. L. Kwok, and F. Mandl, Proc. Phys. Soc. (London) 84, 477 (1964).

provided $\mathbf{A}_{rr}^{-1}$ exists. Note that[17] considerable care should be exercised in deriving results of this type because, in general, $\mathbf{X}$ is a projector and does not have an inverse.

Regrouping the terms above allows (b) to be separated as

$$\mathcal{G}(b)=\mathcal{G}_r(b)+\sum_{p,q}|\,g_p\rangle[(\mathbf{A}_{MM}-\mathbf{A}_{Mr}\mathbf{A}_{rr}^{-1}\mathbf{A}_{rM})^{-1}]_{pq}\times\langle\tilde{g}_q\,|, \quad \text{(C4)}$$

wherein

$$\mathcal{G}_r(b)\equiv\sum_{l,k}|\,l\rangle(\mathbf{X}\mathbf{A}_{rr}^{-1})_{lk}\langle\tilde{k}\,|,$$

$$|\,g_p\rangle\equiv|\,p\rangle-\sum_l|\,l\rangle(\mathbf{A}_{rr}^{-1}\mathbf{A}_{rM})_{lp}, \quad \text{(C5)}$$

$$\langle\tilde{g}_q\,|\equiv\langle\tilde{q}\,|-\sum_l(\mathbf{A}_{Mr}\mathbf{A}_{rr}^{-1})_{ql}\langle\tilde{l}\,|,$$

so that $\mathcal{G}_r(b)$ determines the contribution from distant levels (which, in principle, is a slow function of energy) and the remaining term involves the nearby levels including the effects of distant levels. When the basis states are orthogonal solutions of a Hamiltonian H_0 with homogeneous boundary conditions specified by $\mathfrak{L}^0$, the above formulas easily reduce to those of Refs. 1 and 2. The R matrix is obtained by inserting Eq. (C4) in

$$R_{cc'}(b)=(\hbar^2a_c/2m_c)^{1/2}(\hbar^2a_{c'}/2m_{c'})^{1/2}\times\langle r_c^{-2}\delta(r_c-a_c)c\,|\,\mathcal{G}(b)|\,c'\delta(r_{c'}-a_{c'})r_{c'}^{-2}\rangle. \quad \text{(C6)}$$

Of particular interest is the "single-level" formula, i.e., $M=i=1$, where

$$R_{cc'}(b)=R_{cc'}{}^r(b)+\alpha_{ic}\alpha_{ic'}[\langle\tilde{\imath}\,|\,A\,|\,i\rangle-\sum_{k,l}\langle\tilde{\imath}\,|\,A\,|\,l\rangle(\mathbf{A}_{rr}^{-1})_{lk}\langle\tilde{k}\,|\,A\,|\,i\rangle]^{-1}$$

in which

$$\alpha_{ic}\equiv(\hbar^2a_c/2m_c)^{1/2}\langle r_c^{-2}\delta(r_c-a_c)c\,|[|\,i\rangle-\sum_l|\,l\rangle\times(\mathbf{A}_{rr}^{-1}\mathbf{A}_{rM})_{li}]$$
$$=\gamma_{ic}-\sum_l\gamma_{lc}(\mathbf{A}_{rr}^{-1}\mathbf{A}_{rM})_{li}, \quad \text{(C7)}$$

with the γ_{nc} being the conventional reduced width amplitudes. If one chooses the b_c to be those of the state $|\,i\rangle(=b_{ic}$ say), then the above results when $(H-E_i)|1\rangle=0$ differ from the usual orthogonal theory, i.e., with $\langle\tilde{\imath}\,|\,i\rangle=1$

$$R_{cc'}(b_i)=R_{cc'}{}^r(b_i)+\alpha_{ic}\alpha_{ic'}\times[(E_i-E)-(E_i-E)^2\sum_{l,k}\langle\tilde{\imath}\,|\,k\rangle(\mathbf{A}_{rr}^{-1})_{kl}\langle\tilde{l}\,|\,i\rangle]^{-1}$$

with

$$\alpha_{ic}=\gamma_{ic}-(E_i-E)\sum_{l,k}\gamma_{lc}(\mathbf{A}_{rr}^{-1})_{lk}\langle\tilde{\imath}\,|\,k\rangle.$$

This reduces to the usual R matrix only when $\langle\tilde{\imath}\,|\,k\rangle=0$, although

$$R_{cc'}(b_i)\longrightarrow\frac{\gamma_{ic}\gamma_{ic'}}{E_i-E} \qquad \text{as } E_i\longrightarrow E.$$

Consequently, both approaches (nonorthogonal and orthogonal) yield the same R-matrix behavior very near to the eigenenergy E_i. However, at large values of E_i-E, the nonorthogonal "resonance term" approaches a finite value

$$R_{cc'}(b_i)-R_{cc'}{}^r(b_i)\longrightarrow\beta_{ic}\beta_{ic'}\lambda_i^{-1} \qquad \text{as } |\,E_i-E\,|\longrightarrow\infty,$$

where

$$\beta_{ic}\equiv\sum_{l,k}\gamma_{lc}(\mathbf{A}_{rr}^{-1})_{lk}\langle\tilde{\imath}\,|\,k\rangle,$$

$$\lambda_i\equiv\sum_{l,k}\langle\tilde{\imath}\,|\,l\rangle(\mathbf{A}_{rr}^{-1})_{lk}\langle\tilde{\imath}\,|\,k\rangle,$$

rather than zero as is the case for the orthogonal R matrix.