⁵A. J. F. Siegert, Phys. Rev. <u>52</u>, 787 (1937).

⁶R. G. Sachs and N. Austern, Phys. Rev. 81, 705 (1951).

⁷L. Foldy, Phys. Rev. 92, 178 (1953).

⁸C. Moller and L. Rosenfeld, Kgl. Danske Videnskab.

Selskab, Mat.-Fys Medd. 20, No. 12 (1943).

⁹M. Chemtob and M. Rho, Nucl. Phys. <u>A163</u>, 1 (1971). ¹⁰H. Ohtsubo, J. Fujita, G. Takeda, Progr. Theoret. Phys. 44, 1596 (1970).

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¹¹F. Zachariasen, Phys. Rev. <u>101</u>, 371 (1956).

¹²F. C. Michel, Phys. Rev. B133, 329 (1964).

¹³B. H. J. McKeller, Phys. Letters 26B, 107 (1967).

¹⁴E. M. Henley, to be published; and Phys. Rev. Letters

27, 542 (1971).

¹⁵L. Schülke, Nucl. Phys. B40, 386 (1972).

¹⁶M. Gari, O. Dumitrescu, F. G. Zabolitzky, H. Kummel, Phys. Rev. Letters 35B, 19 (1971).

¹⁷O. Dumitrescu, M. Gari, H. Kummel, F. G. Zabolitzky, Z. Naturforsch. 27a, 733 (1972).

¹⁸M. Gari, Z. Physik 231, 412 (1970).

¹⁹N. Vinh Mau, Lecture given at the Symposium on Nucleons and Weak Interactions, Zagreb, Yugoslavia, July, 1971.

²⁰P. Vogel, California Institute of Technology Report No. CALT-63-155 (unpublished).

²¹A. Bohr and B. Mottelson, Neutron Capture, Gamma Ray Spectroscopy (International Atomic Energy Agency, Vienna, Austria, 1969).

²²G. E. Brown, Nucl. Phys. <u>57</u>, 339 (1964).

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Optimal Nuclear Single-Particle Potential*

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Subject to the validity of the K-matrix approximation for atomic nuclei, it is shown that the best single-particle wave functions are obtained from a self-consistent potential with rearrangement terms. These terms are derived from variational calculus and it is demonstrated that the solution of the Euler-Lagrange equations provides the single determinant wave function with maximal overlap with the true wave function. We solve the equation for the rearrangement term due to the removal of one particle and show that all K matrix elements are on the energy shell.

I. INTRODUCTION

Despite progress in our understanding of nuclear structure, no satisfactory answer has been found for the question: What is the shell-model potential in terms of fundamental theoretical concepts? The binding energy of finite nuclei is calculated using the Brueckner reaction matrix¹: however. there is no undisputed criterion established for choosing or calculating the best single-particle potential for finite-system wave functions and intermediate-state spectra.

In another paper,² we discuss three different choices for the potential which have been made in the literature. We show how their eigenvalues differ due to rearrangement effects, and how each could be observed with varying degrees of difficulty. In the present paper, we show that one choice, that of Brueckner and Goldman,³ has the following advantages:

(1) It is "optimal" in that it follows from a variational theorem that applies under conditions specified here. This potential choice gives the single determinant for which the Brillouin condition⁴ of Brueckner's theory holds. This wave function therefore has maximum overlap with the true wave function.

(2) It is the potential which has eigenvalues equal to separation-energy thresholds. It is thus the choice in accordance with the Landau-Migdal quasiparticle theory, 5, 6 and is most closely related to the phenomenological shell model and the Nilsson-Strutinsky prescription.⁷

(3) When the rearrangement effects due to the re-

moval of one particle are considered, the potential is unambiguously defined with all K matrix elements on the energy shell.

We assume that the hole-line expansion with Kmatrix renormalization for the binding energy of the nucleus converges. We also make the original and natural choice for the particle potential – a continuation of the hole-potential above the Fermi sea for both bound and continuum states. It is necessary to specify the particle energies; otherwise, as has been shown with a counter example (the Lipkin model⁸), any answer for the binding energy may be obtained⁹ unless, of course, the calculation includes all diagrams. Also, no artificial gap in the single-particle intermediate spectrum is thereby introduced as this may also lead to difficulties.¹⁰

II. VARIATIONAL PRINCIPLE

To lowest order in the hole-line expansion, the energy of the nucleus is

$$E = \langle \Phi_0 | T + \frac{1}{2} K[\Phi_0] | \Phi_0 \rangle, \qquad (II.1)$$

where $|\Phi_0\rangle$ is a single-determinant, model wave function. Because we do not prove that *E* is the expectation value of the Hamiltonian in a space of admissible wave functions, it is not obvious that a Rayleigh-Ritz variational minimum can be obtained from this expression. However, supported by recent findings^{10a} and by analogy with the ordinary Hartree-Fock theory, we may minimize the above expression with respect to Φ_0 variations in

our problem, yields

$$\left\{ \left. \mathcal{E} \right| L \right\}_n(i) = \left\{ \left. e \right| L(K_1) \right\}_n(i) + \int di_1 \frac{\partial L}{\partial K_1}(i_1) \left\{ \left. \mathcal{E} \right| g_1^* \right\}_n(i) \right\}_n(i),$$

where

$$\left\{\mathcal{E} \mid g_1^*\right\}_n(i) = \left\{ e \mid g_1^*(K_2) \right\}_n(i) + \int di_2 \, \frac{\partial g_1^*}{\partial K_2}(i_2) \left\{\mathcal{E} \mid (K_2\delta)^* \right\}_n(i)$$
(II.6)

so that

$$\left\{\mathcal{E} \mid L\right\}_{n}(i) = T(i) + \frac{1}{2}K_{1}[i,n] + \frac{1}{2}\int di_{1}n(i_{1})K_{2}[i,i_{1},n] + \int di_{2}n(i_{2})\left\{\mathcal{E} \mid (K_{2}\delta)^{*}\right\}_{n}(i)$$
(II.7)

$$= T(i) + K_1[i, n] + \frac{1}{2} \int di_1 di_2 \{ \mathcal{E} | (K_2 \delta)^* \}_n(i)$$
(II.8)

and

$$\left\{\mathcal{E}|(K_2\delta)^*\right\}_n(i) = \frac{\delta K_2[i_2, i, n]}{\delta n(i_1)} \,\delta(i_1 - i) = \frac{\partial K_2[i_2, i, n]}{\partial n(i)} , \qquad (\text{II.9})$$

because the variation of $K\delta$ vanishes except at $i_1 = i$. Equations (II.8) and (II.9) are the Euler-Lagrange equations derived by the methods of the variational calculus whose solutions will yield the extremal energy. The third term on the right-hand side of Eq. (II.8) is the rearrangement energy [see Eq. (IV.10)] which we discuss in detail in Sec. IV.

order to obtain self-consistent equations for the single-particle potential and its eigenvalues and eigenfunctions.

The variational problem, as stated by Eq. (II.1), is to find the best single Slater determinant wave function, Φ_0 . Variation in such a space of admissible functions is equivalent to a single-particle density matrix. Therefore, we write the general variational derivative as $\delta/\delta n$.

In the terminology of variational calculus, the "Lagrangian" of the energy expression, Eq. (II.1),

$$E = \int di \ L(i, n, K_1[i, n]), \quad L = n(i) \{ T(i) + \frac{1}{2} K_1[i, n] \}$$
(II.2)

involves a functional operator K_1 (the potential energy)

$$K_{1}[i,n] = \int di_{1}g_{1}(i,i_{1},n(i_{1}),K_{2}[i,i_{1},n]),$$

$$g_{1} = n(i_{1})K_{2}[i,i_{1},n],$$
(II.3)

which in turn depends on functional operators K_2 (the reaction matrix K)

$$K_{2}[i, i_{1}, n] = \int di_{2} K_{2}[i, i_{2}, n] \delta(i_{1} - i_{2}),$$

$$K_{2} = K_{ii', ii'}[n] - K_{ii', i'i}[n].$$
(II.4)

Determination of the variational derivative $\delta E/\delta n$ then requires a generalization of Edelen's theorem¹¹ to a multistep "chain rule." (We conjectured this generalization; Edelen¹² furnished the proof given in the Appendix.) Applying this to

(II.5)

III. OPTIMAL WAVE FUNCTIONS

Now we show that, because the resulting eigenfunctions and eigenvalues are the true variationally stable solutions, optimal determinantal wave functions have been found that fulfill a generalized Brillouin⁴ condition.

As discussed in Sec. II, equivalent to the variational derivative with respect to the density, the most general variation of a single determinant is to add particle-hole excitations. Then, in the usual Hartree-Fock derivation, it follows that, at the variational minimum,

$$\delta \langle \Phi_0 | T + \frac{1}{2} v | \Phi_0 \rangle = \langle \delta \Phi_0 | T + \frac{1}{2} v | \Phi_0 \rangle = 0.$$
 (III.1)

Then, if Φ_{ph} is a particle-hole excitation of Φ_0 ,

$$\langle \Phi_{\rm ph} | v | \Phi_0 \rangle = 0 . \tag{III.2}$$

This is the "classical" Brillouin condition.⁴ However, if the interaction v is replaced by the reaction matrix, the above proof holds only if the reaction matrix is held fixed in variationally determining wave functions.¹³ In other words, if the variationally determined wave functions are substituted back into the reaction matrix for self-consistency, the Brillouin theorem is no longer satisfied unless the changes in the reaction matrix are included in the original variation. Note: The formal exact self-consistent field method used by Kobe¹⁴ to show that maximal-overlap wave functions could be obtained without the rearrangement terms does not apply to realistic (approximate) reaction operators.¹³

In the reference-spectrum method,¹⁵ the intermediate-particle spectrum is not made self-consistent. It provides a prescription for calculating the energy, but clearly does not determine selfconsistent single-particle densities. A discussion of the exact self-consistent field theory and reference-spectrum method in this context is given in another paper.¹³

The changes in the reaction matrix fall into two categories, usually symbolized by their first order, the Brueckner-Goldman³ rearrangement diagrams. [See Figs. 1(a), 1(b), and 1(c).] The general variation of

$$K = v + v \frac{P}{e} K$$
(III.3)

yields

$$\delta K = v \frac{\delta P}{e} K + v \frac{P}{e} \delta e \frac{P}{e} K + v \frac{P}{e} \delta K$$
$$= K \frac{\delta P}{e} K + K \frac{P}{e} \delta e \frac{P}{e} K, \qquad (III.4)$$

where the first term is due to the shift induced in

the Pauli operator, and the second is due to the shift induced in the spectrum. (This is worked out in detail in Sec. IV.)

Because variations in K are included, the Φ_0 determined from Eq. (II.8) satisfy the Brillouin condition in the Brueckner theory,

$$\langle \Phi_{\rm ph} | K | \Phi_0 \rangle = 0 . \tag{III.5}$$

Then it follows^{14, 16} that the requirement that

 $\langle \Psi | \Phi_0 \rangle$ = maximum

or

$$\|\Psi - \Phi_0\| = \min(11.6)$$

is equivalent to

$$\langle \Phi_{\rm ph} | t | \Phi_0 \rangle = 0$$
 (III.7)

Here t is the "exact" many-body reaction matrix. Therefore, in so far as K is the "best" approximation to t, the single-particle potential with rearrangement gives the single-determinant wave function with maximum overlap with the true wave function.

IV. SOLUTION FOR THE REARRANGEMENT ENERGY

In order to solve for the rearrangement energy from Eqs. (II.8) and (III.4), let us be more explicit in the equations. The ground-state energy from Eq. (II.1) is

$$E = \sum_{i} n_{i} T_{i} + \frac{1}{2} \sum_{i,j} n_{i} n_{j} (K_{ij, ij} - K_{ij, ji}), \qquad (II.1a)$$

where n_i is the occupation probability for the *i*th level. From Eqs. (II.8) and (II.9),

$$\epsilon_{\alpha} = \frac{\delta E}{\delta n_{\alpha}} \,. \tag{IV.1}$$

Then

$$\epsilon_{\alpha} = \epsilon_{\alpha}^{(1)} + \frac{1}{2} \sum_{i,i} n_i n_j \frac{\delta}{\delta n_{\alpha}} (K_{ij,ij} - K_{ij,ji}), \quad (IV.2)$$

with

$$\epsilon_{\alpha}^{(1)} = T_{\alpha} + \sum_{j} n_{j} (K_{\alpha j, \alpha j} - K_{\alpha j, j \alpha}). \qquad (IV.3)$$

The $\epsilon_{\alpha}^{(1)}$'s are the unrearranged eigenvalues which are equal to a centroid of states in the nucleus with either a hole or particle created in the α th level.² The ϵ_{α} is equal to the separation-energy threshold for removal of the α th particle. It is the eigenvalue prescribed by the Landau-Migdal many-body theory.^{5, 6}

Recall

$$K_{ij, kl} = v_{ij, kl} + \sum_{ab} v_{ijab} \frac{(1 - n_a)(1 - n_b)}{e_i + e_j - e_a - e_b} K_{abkl} ,$$
(III.3a)

where the e's are unspecified at this stage. It follows that

$$\frac{\delta K_{ij,kl}}{\delta n_{\alpha}} = -2\sum_{a} K_{ija\alpha} \frac{1-n_{a}}{e_{i}+e_{j}-e_{a}-e_{\alpha}} K_{a\alpha kl} - \sum_{ab} K_{ijab} \left[\frac{(1-n_{a})(1-n_{b})}{(e_{i}+e_{j}-e_{a}-e_{b})}\right]^{2} K_{abkl} \frac{\delta}{\delta n_{\alpha}} (e_{i}+e_{j}-e_{a}-e_{b}).$$
(IV.4)

(Exchange terms will no longer be written explicitly.) Substituting Eq. (IV.4) into Eq. (IV.2) yields the rearrangement energy

$$\Delta_{\alpha} = \epsilon_{\alpha} - \epsilon_{\alpha}^{(1)} \tag{IV.5}$$

which contains contributions from changes in: (1) the occupation function, (2) the single-particle energies, and (3) the wave functions which appear in the matrix elements.

Equation (IV.4) is only an implicit equation because $\delta e/\delta n_{\alpha}$ depends on $\delta K/\delta n_{\alpha}$. To determine the rearrangement energy for the removal of one particle, neglecting effects from the removal of two or more, we choose the *e*'s to be given by Eq. (IV.3), and the *n*'s to be 1 for occupied states and 0 for unoccupied states. Then

$$\frac{\delta \epsilon_i^{(1)}}{\delta n_{\alpha}} = K_{i\,\alpha,\,i\,\alpha} + \sum_j n_j \frac{\delta K_{ij,\,ij}}{\delta n_{\alpha}};$$
(IV.6)

and

$$\frac{\delta K_{ijkl}}{\delta n_{\alpha}} = -2 \sum_{a} K_{ija\alpha} \frac{(1-n_{a})}{e_{i}+e_{j}-e_{a}-e_{\alpha}} K_{a\alpha kl}$$

$$-2 \sum_{ab} K_{ijab} \frac{(1-n_{a})(1-n_{b})}{e_{i}+e_{j}-e_{a}-e_{b}} \left(K_{i\alpha i\alpha} - K_{a\alpha a\alpha} \right) \frac{(1-n_{a})(1-n_{b})}{e_{i}+e_{j}-e_{a}-e_{b}} K_{abkl}$$

$$-2 \sum_{ab} K_{ijab} \frac{(1-n_{a})(1-n_{b})}{e_{i}+e_{j}-e_{a}-e_{b}} \left[\sum_{b} n_{b} \left(\frac{\delta K_{ipib}}{\delta n_{\alpha}} - \frac{\delta K_{apab}}{\delta n_{\alpha}} \right) \right] \frac{(1-n_{a})(1-n_{b})}{e_{i}+e_{j}-e_{a}-e_{b}} K_{abkl} .$$
(IV.7)

By substituting Eq. (IV.7) into Eqs. (IV.5) and (IV.2) and solving for $\sum_{ij} n_i n_j \, \delta K_{ij,ij} / \delta n_{\alpha}$, the following expression for the rearrangement energy in terms of K is obtained:

$$\begin{split} \Delta_{\alpha} &= -\sum_{ij} n_{i} n_{j} \left(\left\{ \sum_{a} K_{ija\alpha} \frac{(1-n_{a})}{e_{i}+e_{j}-e_{a}-e_{\alpha}} K_{a\alpha ij} + \sum_{ab} K_{ijab} \left(\frac{(1-n_{a})(1-n_{b})}{e_{i}+e_{j}-e_{a}-e_{b}} \right)^{2} K_{abij} \right. \\ & \times \left[K_{i\alpha i\alpha} - K_{a\alpha a\alpha} + 2 \sum_{a''m} n_{m} K_{ama''\alpha} \frac{(1-n_{a''})}{-e_{a}+e_{m}-e_{a''}-e_{\alpha}} K_{a''\alpha am} \right. \\ & + \sum_{m} n_{m} \sum_{a''b''} K_{ama''b''} \left(\frac{(1-n_{a'})(1-n_{b''})}{-e_{a}+e_{m}-e_{a''}-e_{b''}} \right)^{2} (K_{m\alpha m\alpha} - 2K_{a''\alpha a''\alpha}) K_{a''b''am} \right] \right\} \\ & \times \left\{ 1 - 2 \sum_{m} n_{m} \sum_{ab} K_{imab} \left(\frac{(1-n_{a})(1-n_{b})}{e_{i}+e_{m}-e_{a}-e_{b}} \right)^{2} K_{abim} \\ & - 2 \sum_{mm'} n_{m} n_{m'} \sum_{ab} K_{mm'ab} \left(\frac{(1-n_{a})(1-n_{b})}{e_{i}+e_{j}-e_{a}-e_{b}} \right)^{2} \sum_{a''b''} K_{aia''b''} \left(\frac{(1-n_{a''})(1-n_{b''})}{-e_{a}+e_{m}-e_{a''}-e_{b''}} \right)^{2} K_{a''b''ai} K_{abmm'} \left\{ \frac{(1)}{e_{i}+e_{j}-e_{a}-e_{b}} \right\}^{2} \sum_{a''b''} K_{aia''b''} \left(\frac{(1-n_{a''})(1-n_{b''})}{(1-e_{a}+e_{m}-e_{a''}-e_{b''})} \right)^{2} K_{a''b''ai} K_{abmm'} \left\{ \frac{(1)}{e_{i}+e_{j}-e_{a}-e_{b}} \right\}^{2} \sum_{a''b'''} K_{aia''b''} \left(\frac{(1-n_{a''})(1-n_{b''})}{(1-e_{a}+e_{m}-e_{a''}-e_{b''})} \right)^{2} K_{a''b''ai} K_{abmm'} \left\{ \frac{(1)}{e_{i}+e_{j}-e_{a}-e_{b}} \right\}^{2} \sum_{a''b'''} K_{aia''b'''} \left(\frac{(1-n_{a''})(1-n_{b''})}{(1-e_{a}+e_{m}-e_{a''}-e_{b'''})} \right)^{2} K_{a''b''ai} K_{abmm'} \left\{ \frac{(1)}{e_{i}+e_{j}-e_{a}-e_{b}} \right\}^{2} K_{a''b'''ai} K_{a''b'''ai} K_{abmm'} \left\{ \frac{(1)}{e_{i}+e_{j}-e_{a}-e_{b}} \right\}^{2} K_{a''b'''ai} K_{a''b'''ai} K_{abmm'} \left\{ \frac{(1)}{e_{i}+e_{j}-e_{a}-e_{b}} \right\}^{2} K_{a''b'''ai} K_{a''b'''ai} K_{a''b'''ai} K_{a''b'''ai} K_{a''b'''ai} K_{a''b'''ai} K_{a''b'''ai} K_{a''b'''ai} K_{a$$

The six terms in the numerator are presented diagrammatically in Fig. 1 for the hole-rearrangement energy. The equation for Δ_{α} applies equally well to particles. Care must be taken in determining the energy denominators from the diagrams, but Eq. (IV.8) gives the correct expressions.

Throughout the derivation, all K matrix elements are on the energy shell, in that the starting energy is given by the sum of the energies of either the two initial or final particles in the K matrix ele-

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FIG. 1. (a)-(f) Representative diagrams for the holerearrangement energy.

ment. Thus an unambiguous rearrangement potential is displayed by rewriting Eq. (IV.2)

$$\epsilon_{\alpha} = T_{\alpha} + \sum_{j} n_{j} \left(K_{\alpha j \alpha j} + \frac{1}{2} \sum_{i} n_{i} \frac{\delta K_{ij, ij}}{\delta n_{\alpha}} \right) \quad (IV.9)$$

plus exchanges. The quantity in parentheses is the single-particle potential which: (1) includes rearrangement effects, (2) has eigenvalues equal to separation-energy thresholds, and (3) is variationally stable and provides the optimal wave function.

As pointed out previously,³ the eigenvalues are, in general, complex. This reflects the finite lifetime of the excitations.

The self-consistent eigenvalues in Eq. (IV.2) are equal to those defined in the Landau-Migdal manybody theory^{5, 6} which employs Green's-function techniques. They are the thresholds, i.e., the energy differences between the system before and after particle removal or addition, which appear in the single-particle Green's function. That the best density would be obtained by including rearrangement effects is suggested by the fact that the single-particle density is tested by a physical single-hole propagation and that these methods give a good description of transport properties.¹⁷

V. CONCLUSIONS

We have shown, using variational calculus, that the stable, self-consistent solution for the singleparticle potential which gives the lowest energy and the best wave functions contains rearrangement effects. The only assumption required in the proof was that the reaction matrix, which sums particle-particle ladders only, is a good approximation to the exact nuclear reaction matrix. Clearly, this is an assumption which underlies all the work on the Brueckner many-body theory.

Present estimates¹⁸ for the accuracy of the Kmatrix approximation are based on the size of the wound integral, and suggest an error in the total energy of the order 2-4%. On the other hand, the rearrangement corrections appear to be much larger. Old estimates by Brueckner-Goldman³ and more recent models¹⁹ indicate that the $\delta K/\delta n$ term is about 20-40% of the single-particle energy. A recent discussion of the size of these effects is given by Engelbrecht and Weidenmüller.²⁰

It should be noted that no variational problem exists, and any single-particle basis is acceptable for the *exact* reaction matrix. However, in practice we are forced to make approximations. As a result, the choice of the single-particle potential and intermediate-state spectrum is crucial. Other prescriptions may be successful in calculating some specific property of the nucleus. But the theory discussed here is truly self-consistent and yields an optimal single-particle description.

APPENDIX

We have defined our terminology involving "functionals" and "functional operators" in the Appendix of a recent paper coauthored by two of us.²¹ In the following, we introduce Edelen's^{11, 12} full (nonlocal) Euler-Lagrange operator $\{\mathcal{E} \mid L\}_{\Phi}$ rather than the symbol $\delta J/\delta \Phi$ used previously.

If in the notation of Ref. 11 we are given a functional J that depends on a functional operator K_1 which in turn depends on K_2 etc. up to a point where the series is terminated by an ordinary (local) functional, i.e., if

(0)
$$J[\Phi] = \int dV(x)L(x,\Phi(x),K_1[x,\Phi]),$$

(1)
$$K_1[x,\Phi] = \int dV(x_1)g_1(x,x_1,\Phi(x_1),K_2[x_1,\Phi]),$$

(2) $K_{2}[x_{1}, \Phi] = \int dV(x_{2}) g_{2}(x_{1}, x_{2}, \Phi(x_{2}), K_{3}[x_{2}, \Phi]),$

$$(n-1) \quad K_{n-1}[x_{n-2},\Phi] = \int dV(x_{n-1}) g_{n-1}(x_{n-2},x_{n-1},\Phi(x_{n-1}),K_n[x_{n-1},\Phi]),$$

(n)
$$K_n[x_{n-1},\Phi] = \int dV(x_n) g_n(x_{n-1},x_n,\Phi(x_n)),$$

then we get for the Euler-Lagrange derivative, defined by

$$W[\Phi+h] = W[\Phi] + \int dV(\mu) \{\mathcal{E}|\cdot\}_{\Phi}(\mu)h(\mu) + o(||h||),$$

from the *n*th and (n-1)th relations

$$K_{n-1}[x_{n-2},\Phi+h] = K_{n-1}[x_{n-2},\Phi] + \int dV(x_{n-1}) \{\mathcal{E} | g_{n-1}\}_{\Phi}(x_{n-1})h(x_{n-1}) + o(||h||)$$

Thus, from the (n-2)th relation, we have

$$\begin{split} K_{n-2}[x_{n-2},\Phi+h] - K_{n-2}[x_{n-2},\Phi] &- o(\|h\|) \\ &= + \int dV(x_{n-2}) \Big\{ \frac{\partial g_{n-2}}{\partial \Phi(x_{n-2})} h(x_{n-2}) \frac{\partial g_{n-2}}{\partial K_{n-1}} \int dV(x_{n-1}) \Big\{ \mathcal{E}|g_{n-1}\Big\}_{\Phi}(x_{n-2}) h(x_{n-1}) \Big\} \\ &= \int dV(x_{n-2}) \Big\{ \frac{\partial g_{n-2}}{\partial \Phi(x_{n-2})} + \int dV(x_{n-1}) \frac{\partial \overline{g}_{n-2}}{\partial K_{n-1}} (x_{n-1}) \Big\{ \mathcal{E}|\overline{g}_{n-1}\Big\}_{\Phi}(x_{n-2}) \Big\} h(x_{n-2}) . \end{split}$$

Working up the line then yields

$$\begin{split} \left\{ \mathcal{E} \mid L \right\}_{\Phi}(x) &= \left\{ e \mid L(K_1) \right\}_{\Phi}(x) + \int dV \left(x_1 \right) \frac{\partial L}{\partial K_1} \left(x_1 \right) \left\{ \mathcal{E} \mid \overline{g}_1 \right\}_{\Phi}(x) , \\ \left\{ \mathcal{E} \mid \overline{g}_1 \right\}_{\Phi}(x) &= \left\{ e \mid \overline{g}_1(K_2) \right\}_{\Phi}(x) + \int dV \left(x_2 \right) \frac{\partial \overline{g}_1}{\partial K_2} \left(x_2 \right) \left\{ \mathcal{E} \mid \overline{g}_2 \right\}_{\Phi}(x) , \\ \left\{ \mathcal{E} \mid \overline{g}_{n-1} \right\}_{\Phi}(x) &= \left\{ e \mid \overline{g}_{n-1}(K_n) \right\}_{\Phi}(x) + \int dV \left(x_{n-1} \right) \frac{\partial \overline{g}_{n-1}}{\partial K_n} \left(x_{n-1} \right) \left\{ e \mid \overline{g}_n \right\}_{\Phi}(x) . \end{split}$$

The bars indicate interchange of the *n*th and (n-1)th variable (here in g). If g, in the Little Euler-Lagrange operator $\{e \mid g\}_{\Phi}$ involves derivatives up to the *k*th order in an *l*-dimensional x space; $x = (x_{(1)}, x_{(2)}, \ldots, x_{(1)})$, then

$$\{e \mid g\}_{\Phi} \equiv \sum_{\mu=0}^{R} \sum_{\nu=1}^{L} (-)^{\mu} \frac{\partial^{\mu}}{\partial x_{(\nu)}^{\mu}} \frac{\partial_{g}}{\partial (\partial^{\mu\Phi}/\partial x_{(\nu)}^{\mu})}.$$

For further details see the appendix of Ref. 21.

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¹K. A. Brueckner and C. A. Levinson, Phys. Rev. <u>97</u>, 1344 (1955); K. A. Brueckner, R. J. Eden, and N. C. Francis, *ibid.* <u>98</u>, 1445 (1955); K. A. Brueckner, *ibid.* <u>100</u>, 36 (1955); K. A. Brueckner, J. L. Gammel, and H. Weitzner, *ibid.* <u>110</u>, 431 (1958).

²K. A. Brueckner, H. W. Meldner, and J. D. Perez, Phys. Rev. C 6, 773 (1972).

³K. A. Brueckner and D. T. Goldman, Phys. Rev. <u>116</u>, 424 (1959); 117, 207 (1960).

⁴L. Brillouin, Actualities Sci. Ind., No. 71 (1933); No. 159 (1934).

⁵L. D. Landau, Zh. Eksperim. i Teor. Fiz. <u>30</u>, 1058 (1956); <u>32</u>, 59 (1957); <u>35</u>, 97 (1958) [transl.: Soviet

Phys.-JETP 3, 920 (1956); 5, 101 (1957); 8, 70 (1959)]. ⁶A. B. Migdal, Theory of Finite Fermi Systems and Applications to Atomic Nuclei (Interscience, New York, 1967).

⁷S. G. Nilsson et al., Nucl. Phys. <u>A131</u>, 1 (1969).

- ⁸H. J. Lipkin, N. Meshkov, and A. J. Glick, Nucl. Phys. <u>62</u>, 188 (1965).
- ⁹H. R. Petry and S. Schütte, Phys. Letters <u>38B</u>, 167 (1972).

¹⁰G. A. Baker, Jr., and J. L. Gammel, Phys. Rev. C <u>6</u>, 403 (1972).

^{10a}L. Schäfer and H. A. Weidenmuller, to be published. [See also Nucl. Phys. <u>A174</u>, 1 (1971).] Note that their work on maximum-overlap orbitals deals with the complete hole-line expansion and not just with the K-matrix approximation, resulting in a larger set of diagrams for maximum-overlap potentials.

¹¹D. G. B. Edelen, in Modern Analytic and Computational Methods in Science and Mathematics, edited by

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R. Bellman (Elsevier Publishing Company, Inc., New York, 1969), Vol. 19.

¹²D. G. B. Edelen, private communication.

 $^{13}\mathrm{H.}$ W. Meldner and J. D. Perez, Phys. Rev. C (to be published).

¹⁴D. H. Kobe, Phys. Rev. C <u>3</u>, 417 (1971).

¹⁵H. A. Bethe, B. H. Brandow, and A. G. Petschek, Phys. Rev. 129, 225 (1963).

¹⁶V. H. Smith, W. Kutzelniig, Arkiv Fysik <u>38</u>, 309 (1968).

¹⁷C. J. Pethick, Phys. Rev. <u>177</u>, 399 (1969).

¹⁸B. Brandow, in Lectures in Theoretical Physics High

Energy Collisions of Elementary Particles (Gordon and Breach, New York, 1969), Vol. XII B.

¹⁹H. S. Köhler, Phys. Rev. <u>137</u>, B1145 (1964); Nucl. Phys. <u>88</u>, 529 (1965); <u>A128</u>, 273 (1969); R. L. Becker, Bull. Am. Phys. Soc. <u>15</u>, 1315 (1970); H. W. Meldner, Phys. Rev. <u>178</u>, 1815 (1969); and H. W. Meldner and C. M. Shakin, Phys. Rev. Letters <u>23</u>, 1302 (1969). See also Refs. 6 and 18.

²⁰C. A. Engelbrecht and H. A. Weidenmüller, Nucl. Phys. <u>A184</u>, 385 (1972).

²¹K. A. Brueckner, J. H. Chirico, and H. W. Meldner, Phys. Rev. C <u>4</u>, 732 (1971).

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Proton Capture by ⁷Be and the Solar Neutrino Problem^{*}

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It is shown theoretically that the ${}^{7}\text{Be}(p,\gamma){}^{8}\text{B}$ reaction cross section contains substantial contributions from p and d partial waves at laboratory energies, and extrapolations to stellar energies based on the assumption of pure *s*-wave capture are therefore erroneous. However, there is no change in the predicted solar neutrino flux, because the calculated low-energy cross-section factor, 31 eV b, is essentially the same as the empirical value in current use.

I. INTRODUCTION

The recent experiments of Davis¹ have set an upper limit of 1.0 SNU on the neutrino flux from the sun (1 SNU = 10^{-36} captures per target atom per sec), in sharp disagreement with the theoretical prediction of 9 SNU, calculated by Bahcall and Ulrich.² The rare termination of the p-p chain ⁷Be- $(p,\gamma)^{8}B(e^{+}\nu)2\alpha$ results in energetic neutrinos and is calculated to contribute 7.3 SNU. It is therefore important to have an accurate estimate of the rate of this reaction in the solar interior. Very detailed measurements of the cross section for ⁷Be $(p,\gamma)^{8}$ B have been carried out by Kavanagh *et* al.³ (see Barnes⁴) at laboratory energies $E_{b} = 0.165$ to 10.0 MeV. A theoretical extrapolation to lower energies based on a calculation by Tombrello⁵ yielded a zero-energy cross-section factor⁶ S(0)of 0.034 keV b, where, if σ is the cross section and E_{b} the lab proton energy in MeV,

$$S(E_{b}) = 0.87441 \sigma E_{b} \exp(3.9734 E_{b}^{-1/2})$$

for the ⁷Be(p, γ)⁸B reaction. A calculation by Aurdal⁷ similar to that of Tombrello gave S(0) = 0.044 keV b, but the new data of Kavanagh *et al.* were not used in that extrapolation. The value S(0) = 0.030 keV b actually adopted by Bahcall and Ulrich² is lower than either of these, and is presumably the result of an empirical extrapolation.

Proton capture by ⁷Be involves the radiative transition of a proton in a continuum state to the 2⁺ ground state of ⁸B, bound by 137.2 keV. Only dipole radiation is of importance at the energies considered here. Because the spin and parity of ⁷Be are $\frac{3}{2}$, capture from the s and d partial waves leads to E1 radiation, and from the p wave, M1. Higher partial waves cannot contribute to dipole radiation. The calculations of Tombrello⁵ and Aurdal⁷ assumed that only s-wave capture was significant. The present work shows that while this is approximately true in the solar environment $(E_b \approx 20 \text{ keV})$, it is not the case at laboratory energies, even as low as 150 keV. The small binding energy of ⁸B results in a spatially extended wave function, enhancing capture from the p and d partial waves.

II. DERIVATION OF THE CROSS SECTION

The total cross section for dipole capture in the reaction $A(a, \gamma)B$ is

$$\sigma_1 = (16/9)\pi E_{\gamma^3}(\hbar c)^{-4} (M_a c^2/2E_a)^{1/2} \\ \times \sum_{\mu \, mM_A \, M_B} (2s+1)^{-1} (2J_A+1)^{-1} |T_1^{\mu}|^2,$$