LA-UR -81-403

CONF-810107--2

TITLE: EFFECTIVE HAMILTONIAN THEORY: RECENT FORMAL RESULTS AND NON-NUCLEAR APPLICATIONS

AUTHOR(S): B. H. Brandow

MASTER

TO APPEAR IN: "Proceedings of the Second International Conference on Recent Progress in Many-Body Theories," (Mexico, January 1981)

University of California

LOS ALAMOS SCIENTIFIC LABORATORY
Post Office Box 1663 Los Alamos, New Mexico 87545
An Affirmative Action/Equal Opportunity Employer

Form No. 836 R3
St. No. 2629
12/78

UNITED STATES
DEPARTMENT OF ENERGY
CONTRACT W-7405-ENG. 36

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

EFFECTIVE HAMILTONIAN THEORY: RECENT FORMAL RESULTS AND NON-NUCLEAR APPLICATIONS*

B. H. Brandow
Theoretical Division
Los Alamos National Laboratory
University of California
Los Alamos, NM 87545

I. Introduction

Effective Hamiltonian theory is actually quite an old subject, dating back to a 1929 paper of Van Vleck,[1] and a subsequent refinement by Kemble.[2] Their approach, the so-called canonical transformation or unitary transformation method, is widely known throughout all branches of quantum physics, from high-energy theory to quantum chemistry. The alternative is to use degenerate perturbation theory. This is available in several different forms, most notably those of Kato,[3] Bloch,[4] and des Cloizeaux.[5] The past 15 years have seen an intensive development of the subject by nuclear physicists,[6-8] based on one of these forms of degenerate perturbation theory.

At first sight, the various degenerate perturbation formalisms all seem more complicated than the unitary approach, their interrelations seem rather obscure, and moreover they seem totally unrelated to the unitary method. It is now recognized, however, that most of the perturbative formalisms which lead to Hermitean effective Hamiltonians are, in fact, completely equivalent, and are connected by simple identities.[9-11] We will focus here on a point which is far less obvious: the fact that, subject to an important caveat, these Hermitean perturbation formalisms are actually identical, term-by-term, to the unitary transformation approach, when the latter's effective Hamiltonian is expanded as a perturbation series. The study of this connection also has the important benefit of revealing the relative merits of these approaches for practical applications. The conclusion is that the approach familiar to nuclear physicists is by far the most powerful and efficient one, especially for many-body applications.

Another important recent development concerns the coupled-cluster formalism for many-body systems. This form of many-body theory was originally developed by Coester and Kümmel[12] for closed-shell systems. Over the years, both Coester[13] and Kümmel and coworkers[14] have worked on extensions to open-shell systems, and Zabolitzky and Ey[15] have done some highly sophisticated nuclear calculations using this approach. Quite recently, however, Lindgren[16] has developed a beautifully clean formulation of the coupled-cluster method for open-shell systems. Although not essentially different from the previous work, it has the important pedagogical advantages of being clear, concise, and quite general. We shall outline the main features of Lindgren's formula-

---

*Work supported by US Department of Energy

tion. This alternative to perturbation theory may well be advantageous for certain systems, as it suggests different classes of approximations;[17] it certainly deserves much further development.

Although the many-body linked-cluster form of degenerate perturbation theory was first developed for nuclear physics applications,[6-8] it is clear that this is, in fact, a very general technique for deriving effective Hamiltonians for the low-energy excitations of any many-fermion system. (This formalism has also been extended to handle the elementary excitations of the boson system of liquid ^{4}He.[18]) I shall briefly describe three recent applications where this formalism has contributed significantly to the understanding of other many-body systems. These applications are (a) the derivation of effective spin Hamiltonians in magnetic insulator systems; (b) derivation and ab initio calculation of effective π-electron Hamiltonians for planar conjugated hydrocarbon molecules, and (c) understanding the so-called valence fluctuation phenomenon exhibited by certain rare-earth compounds.

The present formal matters are reviewed in considerably more detail in Ref. 11, together with application (b). Application (a) is covered in depth in Ref. 19, whereas application (c) is quite new, and is yet only partially published.[20]

II. Degenerate Perturbation Theory

We shall first outline what we regard as the most simple and efficient formulation of degenerate perturbation theory. We present only the key equations, and refer the reader to Ref. 11 for further details.

The simplest version of degenerate perturbation theory is the Brillouin-Wigner form, where the effective interaction matrix is $P\mathcal{V}P$, and $\mathcal{V}$ is determined fro

$$\mathcal{V} = VP + \frac{Q}{e}\mathcal{V} = V\sum_{n=0}^{\infty}\left(\frac{Q}{e}V\right)^n P \equiv V\Omega \quad . \qquad (2.1)$$

Here P and Q are the usual projection operators onto the "model" and "virtual" subspaces ($P + Q = I$), $H = H_0 + V$, and $e \doteq E - H_0$. The effective Hamiltonian of this formulation is $P(H_0 + \mathcal{V})P$. Its eigenvalues E are identical to certain eigenvalues of the complete Hamiltonian H, and its eigenvectors represent the "model projections" $P\Psi$ of the corresponding complete eigenvectors Ψ. For later use we have also introduced the wave operator Ω, which has the property that $\Psi = \Omega(P\Psi)$.

From a practical standpoint, this formulation has three serious drawbacks. Most obvious is that $\mathcal{V}$ depends on the (initially unknown) eigenvalue E, and furthermore this operator must be re-determined for each of the desired eigenstates with different eigenvalues E. Second, for many-body systems the Brillouin-Wigner expansion (2.1) lacks the important linked-cluster property. (Even for relatively few-body systems this property remains vital; see Ref. 11.) Finally, the above effective Hamiltonian has a non-Hermitean aspect, since its eigenvectors are not mutually orthogonal. (They are merely the projections $P\Psi$ of the complete eigenvectors Ψ.) This is undesireable because the various phenomenological effective Hamiltonians which one would like to explain are invariably Hermitian.

The first two of these deficiencies can be removed by expanding the energy dependence of $\mathcal{V}$ in a Taylor series. This eventually leads to the implicit equation

$$\mathcal{W} = \sum_{r=0}^{\infty} \mathcal{V}_r \, [-\mathcal{W}]^r , \qquad \mathcal{V}_r = \frac{(-1)^r}{r!} \, P \, \frac{d^r \mathcal{V}}{dE^r}\Big|_{E_0} P \quad . \tag{2.2}$$

This $\mathcal{W}$ replaces $P\mathcal{V}P$ as the effective interaction matrix. The Rayleigh-Schroedinger (RS) expansion for $\mathcal{W}$, i.e. the ordinary power series in V, can now be obtained by first solving (2.2) recursively, in terms of matrix products of the various $\mathcal{V}_r$'s, then replacing the latter by their perturbation series, thus:

$$\begin{aligned} \mathcal{W} &= \mathcal{V}_0 + \mathcal{V}_1 \, [-\mathcal{V}_0] + \mathcal{V}_2 \, [-\mathcal{V}_0]^2 + \mathcal{V}_1 [-\mathcal{V}_1][-\mathcal{V}_0] + \mathcal{O}(\mathcal{V}_r)^4 \\ &= VPV + PV \frac{Q}{e_0} VP + PV \frac{Q}{e_0} V \frac{Q}{e_0} VP + PV \frac{1}{e_0} \frac{Q}{e_0} V(-P) \, VP + \mathcal{O}(V^4) \quad . \end{aligned} \tag{2.3}$$

Here $e_0 \equiv E_0 - H$, and E_0 comes from PH_0P, assuming H_0 exactly degenerate within P. (This restriction is only for simplicity; it can easily be removed.) Finally, $\mathcal{W}$ may be replaced by a "Hermitized" effective interaction matrix,

$$\mathcal{K} = \tfrac{1}{2}[(1 + \Theta)^{\frac{1}{2}} \mathcal{W} (1 + \Theta)^{-\frac{1}{2}} + \text{h.c.}] = \tfrac{1}{2}[\mathcal{W} + \mathcal{W}^{\dagger}] + \mathcal{O}(\Theta) \quad , \tag{2.4}$$

where $\Theta = \Omega^{\dagger} \, Q \, \Omega$ has a well-defined RS expansion which follows from the preceeding equations. This $\mathcal{K}$ operator has the same eigenvalues as $\mathcal{W}$, but its eigenvectors are now precisely orthogonal.

The RS expansion for this $\mathcal{K}$ operator can be generated by several alternative methods,[4,5,11] but the present procedure has significant practical advantages. The expansion (2.1) is obviously a geometric series, and (2.2) also has a geometric-like character [since one is expanding the denominators $(E_0 + \Delta E - H_0)^{-1}$]. One finds, therefore, that (2.1)-(2.3) present many opportunities for infinite partial summation of the series, a technique of great importance for practical applications. (See for example Ref. 8.) The last step (2.4), on the other hand, is by far the most complicated one, from the standpoint of its effect on the structure of the perturbation series. But in all applications to date that we are aware of, the lack of Hermiticity in $\mathcal{W}$ has turned out to be quantitatively quite minor. It should usually, therefore, be quite adequate to use just the "zeroth order" approximation, $\mathcal{K} \approx \tfrac{1}{2}(\mathcal{W} + \mathcal{W}^{\dagger})$. This is a major simplification. The alternative methods for generating the RS expansion for $\mathcal{K}$ have this complicated "Hermitization aspect" inextricably mixed with the other aspects, which therefore severely restricts the possibilities for efficient partial summation.

III. The Unitary Transformation Method

Van Vleck[1] introduced the idea of a unitary transformation of H,

$$\mathcal{H} = U^{-1} H U \quad , \tag{3.1}$$

where U is to be chosen such that

$$Q \mathcal{H} P = 0 \quad . \tag{3.2}$$

The desired effective Hamiltonian is then $P\mathcal{H}P$. Unfortunately, (3.2) does not suffice to determine U or $P\mathcal{H}P$ uniquely, since arbitrary unitary transformations within the P subspace are still allowed. It seems most reasonable to add a requirement that U should have as little effect as possible within the P subspace (and likewise for the Q subspace). Kemble[2] suggested that U should be expressed in a matrix-exponential form,

$$U = e^{G}, \quad G^{\dagger} = -G \quad , \tag{3.3}$$

whereby this somewhat vague "minimal effect" requirement can be incorporated via the simple subsidiary conditions

$$PGP = 0, \quad QGQ = 0. \tag{3.4}$$

One may then express G as a formal expansion in powers of V, and collect the resulting terms in $\mathcal{H}$ for each order in V. The condition (3.2) can then be imposed separately for the terms of each order in V [subject also to $G^{\dagger} = -G$ and (3.4)] to determine the successive terms in the G expansion.

The net result of this procedure is to generate a Rayleigh-Schroedinger expansion for the effective Hamiltonian $P\mathcal{H}P$. In common with the preceeding $P(H_0 + \mathcal{X})P$ this should generate some subset of the exact eigenvalues E, but it is not at all obvious whether these two effective Hamiltonians should have the same sets of model eigenvectors. These effective Hamiltonians might well differ by a unitary transformation within P, in which case their perturbative expansions would also be different.

IV. Formal Equivalence of the Perturbative and Unitary Approaches

It turns out that the effective Hamiltonians of Sections II and III are not merely unitarily equivalent; *they are actually identical*. That is, their respective Rayleigh-Schroedinger expansions are identical. This welcome result was first recognized by Klein,[9] and was later proven in a quite different manner by Jørgensen.[31] (Klein's proof unfortunately contains some errors; a corrected proof consists of two parts, given in appendices in Refs. 11 and 19.) In retrospect, one can see that both proofs are based on the idea (Section III) that the transformation from H to the effective Hamiltonian should have "minimal effect within P." The proofs also share a common strategy: a precise definition is given for this "minimal effect," this requirement is shown to have a unique solution, and then each of the effective Hamiltonians is shown to satisfy this requirement.

Jørgensen's proof[21,11] is based on the requirement that PUP should be Hermitean. (To motivate this choice, consider the one-dimensional case where $U = e^{i\theta}$. Here Hermiticity requires that $U = \pm 1$. The -1 possibility is then eliminated by requiring continuity as $V \to 0$.) It turns out that the subsidiary conditions (3.4) are sufficient (although not necessary) to make PUP Hermitean.[11] It is less obvious how to apply this requirement to $P(H_0 + \mathcal{V})P$, since no U is visible here. There are, however, some simple identities[11] which show that

$$P(H_0 + \mathcal{V})P = (\Omega^\dagger\Omega)^{-\frac{1}{2}} \, (\Omega^\dagger H\Omega)(\Omega^\dagger\Omega)^{-\frac{1}{2}}, \tag{4.1}$$

whereby $UP = \Omega(\Omega^\dagger\Omega)^{-\frac{1}{2}}$, and thus $PUP = (\Omega^\dagger\Omega)^{-\frac{1}{2}}$, which is now obviously Hermitean.

Klein's proof is based on the following variational problem: Let $\{\alpha\}$ be the set of d eigenstates which are described by the d-dimensional model Hamiltonian (d = dimension of P), and let $\{\Psi_\alpha\}$ be the corresponding set of complete eigenvectors (eigenvectors of H). Let $\{B_\alpha\}$ be a set of d vectors which lie entirely within P. These B_α's are required to be orthonormal, but are otherwise arbitrary; the infinity of possible choices for $\{B_\alpha\}$ are therefore related by unitary transformations within P. The Ψ_α's are also required, here, to have unit norms, but of course they do <u>not</u> lie entirely within P. The problem is to find the basis set $\{B_\alpha\}$ such that the quantity $\Sigma_\alpha \langle B_\alpha - \Psi_\alpha \; B_\alpha - \Psi_\alpha \rangle$ attains its absolute (i.e. global) minimum. The solution of this vector variational problem is known to be unique,[22,19] and the sets of model eigenvectors of the perturbative and unitary effective Hamiltonians both satisfy this condition (as proven, respectively, in the appendices of Refs. 19 and 11). Finally, since the eigenvalues and eigenvectors of these model Hamiltonians are identical, the operators themselves much be identical.

Jørgensen's proof leads to important insights about the relative merits of the perturbative and unitary approaches. As described in Section III, the unitary approach has a simplicity and elegance which has appealed to generations of physicists. In reality, however, this simplicity is only an illusion. Beyond the lowest orders the recursive procedure for determining G and $P\mathcal{V}P$ becomes exceedingly tedious, and offers no general insights of the type needed for infinite partial summations. Two reasons for this complexity can now be seen. One is that the unitary approach must necessarily include the complicated "Hermitisation aspect" of (2.4). The other is that the perturbation series for $UP = \Omega(\Omega^\dagger\Omega)^{-\frac{1}{2}}$, as determined by the methods of Section II, does not have an exponential-like character, thus it is "unnatural" (i.e. inefficient) to focus on the (matrix) logarithm of U, as is done in the Van Vleck-Kemble approach.

We must not leave this subject without mentioning an important caveat. The original works did not fully specify how the unitary approach is to be implemented in higher orders. We have presumed a single unitary transformation, whose G contains all orders in V. There have been a number of applications, however, which employ a succession of unitary transformations,

$$U' = U_1 \, U_2 \, U_3 \, \text{---} = e^{G_1} \, e^{G_2} \, e^{G_3} \, \text{---} \quad , \tag{4.2}$$

where each transformation enforces (3.2) for one higher order in V. The subsidiary conditions (3.4) are commonly imposed for each of the G_n's. (A well-known example of this procedure is the work of Foldy and Wouthuysen,[23] whose object was to eliminate the small components of the Dirac equation.) Explicit calculation shows that this gives <u>different</u> results from the methods of Sections II and III; specifically, $PU'P - PUP \sim \mathcal{O}(V^3)$ and $P\mathcal{W}'P - P\mathcal{W}P \sim \mathcal{O}(V^4)$. Such differences have sometimes led to confusion, as pointed out by Friar.[24]

V. Coupled-Cluster Formalism for Open-Shell Systems

Elementary manipulation of the Schroedinger equation leads to the operator identity

$$[\Omega, H_o] = V\Omega - \Omega V\Omega \quad . \tag{5.1}$$

(It is to be understood that $\Omega = \Omega P$, i.e., that Ω acts only on the P subspace.) This is one of the two basic ingredients of Lindgren's formulation.[17] His other ingredient refers explicitly to the many-body nature of an open-shell many-fermion system, as follows.

For closed-shell systems, it is well known[6] that the wave operator Ω can be expressed as

$$\Omega = e^{\hat{W}} \quad , \tag{5.2}$$

where $\hat{W} = \Sigma_{n=1}^{N} \hat{W}_n$, N being the total number of particles. Each $\hat{W}_n$ corresponds to the sum of all <u>linked</u> but <u>open</u> perturbation diagrams which lead to the creation of n particle-hole pairs (starting from the closed-shell configuration Φ_o). The caret symbol is a reminder that $\hat{W}$ is a second-quantized operator, with a particle creation or annihilation operator attached to the end of each outgoing particle or hole line associated with an individual $\hat{W}_n$ component amplitude. Lindgren noted that this representation is inadequate for open-shell systems, and that it should be replaced by

$$\Omega = \left\{e^{\hat{W}}\right\} = \sum_{r=0}^{\infty} \frac{1}{r!} \left\{\hat{W}^r\right\} \quad , \tag{5.3}$$

where { } indicates normal-ordering of the various creation and annihilation operators. Failure to do this would lead to many spurious terms.[11] (This point was also recognized by Kümmel and coworkers,[14] but was not clearly stated.)

It is easy to see that systematic use of (5.1) as a recursion formula will generate the Rayleigh-Schroedinger perturbation expansion for Ω. Following this procedure, Lindgren was able to prove by induction that the perturbation-theoretic Ω does indeed have the form (5.3), where each term in $\hat{W}$ is fully connected, and is also "open" in the sense of always leading to states in the Q subspace. (It then follows that $\mathcal{W} = PV\Omega$ is fully linked.) In a similar manner, Lindgren then obtained a formal equation for $\hat{W}$ itself. This translates into an inhomogeneous set of equations for the various cluster amplitudes within $\hat{W}$. If one adopts some suitable (physically motivated) truncation of these equations, it becomes possible to obtain the "most relevant" amplitudes directly, without using perturbation theory. This is the open-shell analog of the coupled-cluster technique.

VI. Recent Non-Nuclear Applications

A. Effective Spin Hamiltonians for Magnetic Insulator Materials

Magnetic insulator materials include nearly all halides, most oxides, and a number of sulphides of the 3d (transition) and 4f (rare earth) metals, as well as some of the 5f (actinide) metals, plus many other ionic compounds of these metals; thousands of examples are known. Their magnetic behaviors can generally be described by effective Hamiltonians of the form

$$\mathcal{H} = -\sum_{ij} J_{ij}\vec{S}_i\cdot\vec{S}_j + \text{small corrections}, \tag{6.1}$$

where the couplings J_{ij} are typically found to be antiferromagnetic and of fairly short range. This is the so-called Heisenberg spin Hamiltonian, and efforts to understand its microscopic origin date back to the late 1920's. The so-called superexchange theory of Anderson[25] is the standard in this field, and gives a good qualitative and semi-quantitative account of the physics. But this theory is restricted to an *isolated pair* of magnetic ions in a non-magnetic host crystal [two Ni's in MgO, two Cr's in Al_2O_3 (= "ruby"), etc.]. *All* previous attempts to extend this (or any other) theory to a crystal with a macroscopic number N of magnetic ions had met with difficulties of the unlinked-cluster type: terms involving high powers of N. This is known historically as the nonorthogonality catastrophe, first observed by Slater[26] in 1930, and it is quite possibly the first unlinked-cluster problem to be recognized since the development of wave mechanics. It was, therefore, quite gratifying to find that the folded-diagram expansion resolves this problem in a clean, general, and complete manner.[19] A curious feature of this application is that the appropriate H_0 now contains two-body as well as one-body terms. Apart from some minor refinements, however, this was simply a matter of embedding Anderson's two-site perturbation theory into the full many-body formalism.

B. π-Electron Hamiltonians

In planar hydrocarbon molecules with double bonds, molecules such as ethylene, benzine, anthracene, etc., the two bonds of a double bond are not equal. One is a *strong* bond composed of so-called σ orbitals (hybrids of carbon 2s, $2p_x$ and $2p_y$ orbitals) which lie *in* the molecular plane, while the other is a *weak* bond involving carbon $2p_z$ orbitals oriented *perpendicular* to the plane, the so-called π orbitals. Pariser, Parr, and Pople[27] showed in 1953 that the lowest few electronic excited states of these molecules can be described fairly accurately by attributing all of the action to just the π electrons alone, with their interactions described by a small number of phenomenological parameters. Moreover, these parameters are quite transferable -- those determined from the optical absorptions of benzine provide good predictions for the corresponding spectra of napthaline, anthracine, and the other "chickenwire" compounds. This scheme has since been extended to much wider classes of molecules, and it is now a standard textbook subject for organic chemists. Nevertheless, many theoretical chemists have rejected this as "dirty phenomenology, with no theoretical justification," and they will have nothing to do with this scheme.

There is, of course, another school of theoretical chemists who have been attacking this problem with various formal techniques, and in recent years their efforts have been evolving towards the folded-diagram expansion of Ref. 6. I am convinced that the latter (or its coupled-cluster counterpart) really is the optimum formalism for the π-electron problem, and I have therefore written some pedagogical reviews[28,11] directed towards these chemists. At the least this provides a sound formal justification for the phenomenology, and efforts are also underway by several investigators to calculate the parameters from "first principles."

C. Valence Fluctuations in Rare Earth Compounds

"Valence fluctuations" is the name of a many-body phenomenon first recognized about ten years ago.[29] It is seen in a number of rare earth compounds, some "classic" examples being SmS, SmB_6, and TmSe. At low temperatures essentially all electronic properties become quite anomalous, indicating a novel type of many-body ground state. The subject is complex and still poorly understood. Suffice it to say that this is closely related to the Kondo effect, and the most popular model for theoretical study is a dense lattice of Kondo-like ions (actually Anderson-Hamiltonian ions) embedded in a simple metal. It is also somewhat analogous to the BCS problem, to the extent that a "zeroth order" description involves an enormous degeneracy, whereby strong cooperative effects can result from a weak residual interaction.

Pursuing this BCS analogy, we constructed simple variational wavefunctions for the ground states of various model systems.[20] The central problem was to evaluate the necessary many-body expectation values, so that parameters could be optimized and the physics extracted. The graphology for the above spin-Hamiltonian problem turned out to be well-suited for this task, and the various expectation values were found to have simple analytic forms. The resulting physical output is consistent with much of the observed phenomenology.

These examples suggest that the effective Hamiltonian formalism has much potential for other fruitful applications.

References

1) J. H. Van Vleck, Phys. Rev. **33**, 467 (1929).

2) E. C. Kemble, *The Fundamental Principles of Quantum Mechanics* (McGraw-Hill, New York, 1937), p. 394.

3) T. Kato, Prog. Theor. Phys. 4, 514 (1949).

4) C. Bloch, Nucl. Phys. **6**, 329 (1958).

5) J. des Cloizeaux, Nucl. Phys. 20, 321 (1960).

6) B. H. Brandow, Rev. Mod. Phys. 39, 771 (1967).

7) Effective Interactions and Operators in Nuclei, B. R. Barrett, ed. (Springer-Verlag, Berlin, 1975).

8) P. J. Ellis and E. Osnes, Rev. Mod. Phys. 49, 777 (1977).

9) D. J. Klein, J. Chem. Phys. 61, 786 (1974).

10) B. H. Brandow, in Ref. 7.

11) B. H. Brandow, Int. J. Quantum Chem. 15, 207 (1979).

12) F. Coester and H. Kümmel, Nucl. Phys. 17, 477 (1960).

13) F. Coester, in Lectures in Theoretical Physics, Vol. 11B, K. T. Mahanthappa and W. E. Brittin, eds. (Gordon & Breach, New York, 1969), p. 157.

14) R. Offermann, W. Ey, and H. Kümmel, Nucl. Phys. A 273, 349 (1976); R. Offermann, Nucl. Phys. A 273, 368 (1976); W. Ey, Nucl. Phys. A 296, 189 (1978).

15) J. Zabolitsky and W. Ey, Nucl. Phys. A328, 507 (1979).

16) I. Lindgren, Int. J. Quantum Chem., Symp. Vol. 12, 33 (1978).

17) J. Paldus, J. Cizek, and I. Shavitt, Phys. Rev A5, 50 (1975).

18) B. H. Brandow, Ann. Phys. (NY) 64, 21 (1971).

19) B. H. Brandow, Adv. Phys. 26, 651 (1977); see §6.5.

20) B. H. Brandow: Int. J. Quantum Chem. 13, 423 (1979); in Crystalline Electric Field and Structural Effects in f-Electron Systems, J. E. Crow, R. P. Guertin, and T. W. Mihalisin, eds. (Plenum, New York, 1980), p. 353; and preprint.

21) F. Jørgensen, Mol. Phys. 29, 1137 (1975), see pp 1144-46; also private communication.

22) B. C. Carlson and J. M. Keller, Phys. Rev. 105, 102 (1967).

23) L. L. Foldy and S. A. Wouthuysen, Phys. Rev. 78, 29 (1950).

24) J. L. Friar: in Mesons in Nuclei, M. Rho and D. H. Wilkinson, eds. (North-Holland Publ. Co., Amsterdam, 1979), see §3; Phys. Rev. C 22, 796 (1980).

25) P. W. Anderson, Phys. Rev. 79, 350 (1959); Solid State Phys. 14, 99 (1963).

26) J. C. Slater, Phys. Rev. 35, 509 (1930).

27) R. Pariser and R. G. Parr, J. Chem. Phys. 21, 466 and 767 (1953); J. A. Pople, Trans. Faraday Soc. 49, 1375 (1953).

28) B. H. Brandow, in Advances in Quantum Chemistry, P.-O. Löwdin, ed. (Academic Press, New York, 1977), p. 188; B. H. Brandow, in Quantum Theory of Polymers, J.-M. André, J. Delhalle, and J. Ladik, eds. (D. Riedel Publ. Co., Dordrecht, 1978).

29) C. M. Varma, Rev. Mod. Phys. 48, 219 (1976).