INTRODUCTION TO THE SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY AND ITS DIAGRAMMATIC REPRESENTATION

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Chemical Sciences, Geosciences
& Biosciences Division

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SHORT COURSE OFFERED DURING THE XINGDA LECTURESHIP VISIT

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MANY THANKS TO PROFESSOR KAI WU AND COMMITTEE FOR ACADEMIC EXCHANGES FOR INVITATION AND PROFESSOR JIAN LIU FOR HOSPITALITY

MANY-PARTICLE SCHRÖDINGER EQUATION

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QUANTUM CHEMISTRY: THE ELECTRONIC SCHRÖDINGER EQUATION

$$H_e \Psi_K(\mathbf{X};\mathbf{R}) = E_K(\mathbf{R}) \Psi_K(\mathbf{X};\mathbf{R})$$

$$H_e = Z + V = \sum_{i=1}^{N} z(\mathbf{x}_i) + \sum_{i>j=1}^{N} v(\mathbf{x}_i, \mathbf{x}_j)$$

$$z(\mathbf{x}_i) = -\tfrac{1}{2}\Delta_i + \sum_{A=1}^{M} \frac{Z_A}{R_{Ai}}, \qquad v(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{r_{ij}}$$

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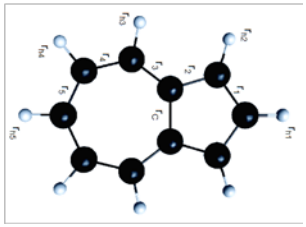

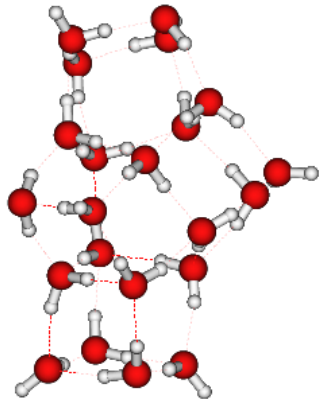

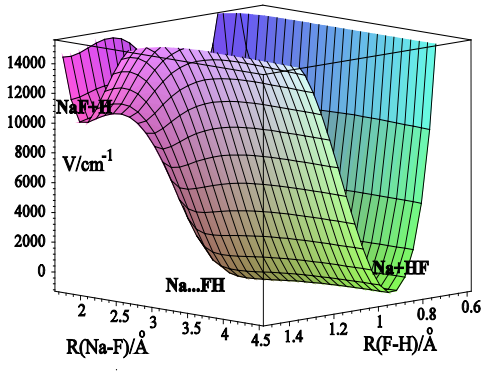

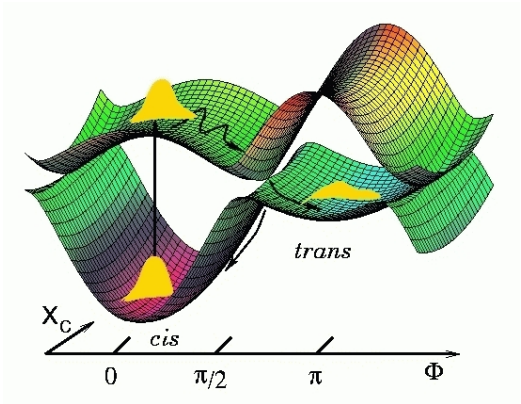

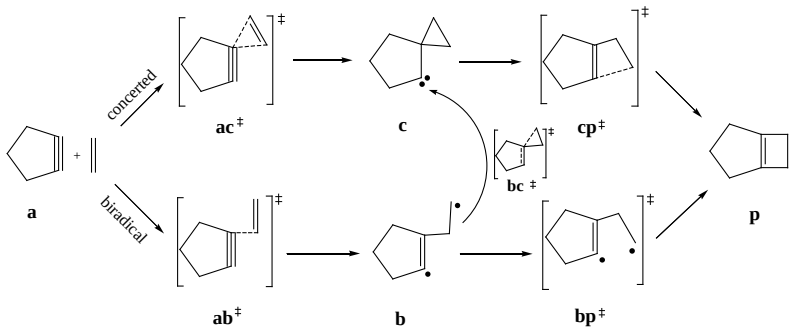

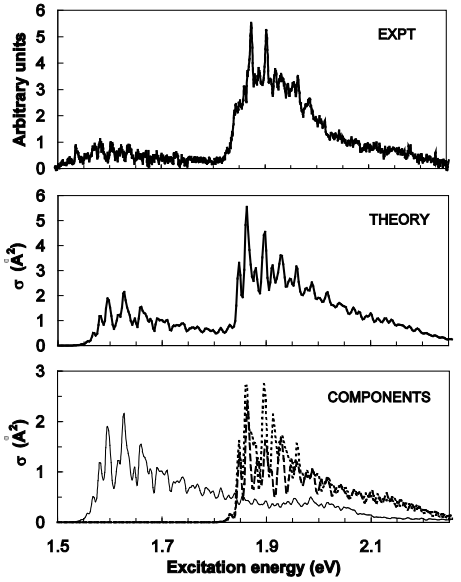

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NUCLEAR PHYSICS: THE NUCLEAR SCHRÖDINGER EQUATION

$$H_n \Psi_\mu(\mathbf{X}) = E_\mu \Psi_\mu(\mathbf{X})$$

$$H_n = Z + V_2 + V_3(+???) = \sum_{i=1}^{N} z(\mathbf{x}_i) + \sum_{i>j=1}^{N} v_2(\mathbf{x}_i, \mathbf{x}_j) + \sum_{i>j>k=1}^{N} v_3(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k)(+???)$$

$$z(\mathbf{x}_i) = \frac{p_i^2}{2m_i}, \quad v_2(\mathbf{x}_i, \mathbf{x}_j) =? \text{ (Argonne } v_{18}\text{, CD Bonn, Idaho-A, etc.)},$$

$$v_3(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k) =? \text{ (Tucson-Melbourne, Urbana IX, etc.)}$$

} or NLO, N^{2}LO, N^{3}LO, etc.

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MANY-BODY TECHNIQUES DEVELOPED IN ONE AREA SHOULD BE APPLICABLE TO OTHER AREAS

SOLVING THE MANY-PARTICLE SCHRÖDINGER EQUATION

- Define a basis set of single-particle functions (e.g., LCAO-type molecular spin-orbitals in quantum chemistry obtained by solving mean-field equations or harmonic oscillator basis in nuclear physics)

$$V \equiv \left\{ \varphi_r(\mathbf{x}), r = 1, \ldots, \dim V \right\}$$

Exact case : $\dim V = \infty$, in practice : $\dim V < \infty$

- Construct all possible Slater determinants that can be formed from these spin-particle states

$$\Phi_{r_1 \ldots r_N}(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{r_1}(\mathbf{x}_1) & \cdots & \varphi_{r_1}(\mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ \varphi_{r_N}(\mathbf{x}_1) & \cdots & \varphi_{r_N}(\mathbf{x}_N) \end{vmatrix}$$

SOLVING THE MANY-PARTICLE SCHRÖDINGER EQUATION

- The exact wave function can be written as a linear combination of all Slater determinants

$$\Psi_\mu(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \sum_{r_1<\cdots<r_N} c^\mu_{r_1\ldots r_N}\Phi_{r_1\ldots r_N}(\mathbf{x}_1,\ldots,\mathbf{x}_N)$$

$$= \sum_I c^\mu_I \Phi_I(\mathbf{x}_1,\ldots,\mathbf{x}_N)$$

- Determine the coefficients *c* and the energies E_μ by solving the matrix eigenvalue problem:

$$\mathbf{HC}^\mu = E_\mu \mathbf{C}^\mu$$

where the matrix elements of the Hamiltonian are

$$H_{IJ} = \left\langle \Phi_I \middle| \hat{H} \middle| \Phi_J \right\rangle = \int d\mathbf{x}_1 \ldots d\mathbf{x}_N \Phi^*_I(\mathbf{x}_1,\ldots,\mathbf{x}_N)\hat{H}\Phi_J(\mathbf{x}_1,\ldots,\mathbf{x}_N)$$

- This procedure, referred to as the full configuration interaction approach (FCI), yields the exact solution within a given single-particle basis set

THE PROBLEM WITH FCI

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Dimensions of the full CI spaces for many-electron systems

	Number of correlated electrons			
Orbitals	6	8	10	12
20	379×10^3	5.80×10^6	52.6×10^6	300×10^6
30	4.56×10^6	172×10^6	4.04×10^9	62.5×10^9
100	6.73×10^9	3.20×10^{12}	9.94×10^{14}	2.16×10^{17}

Dimensions of the full shell model spaces for nuclei

Nucleus	4 shells	7 shells
^{4}He	4E4	9E6
^{8}B	4E8	5E13
^{12}C	6E11	4E19
^{16}O	3E14	9E24

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- Alternative approaches are needed in order to study the majority of many-body systems of interest

The key to successful description of atoms, molecules, condensed matter systems, and nuclei is an accurate determination of the MANY-PARTICLE CORRELATION EFFECTS. INDEPENDENT-PARTICLE-MODEL APPROXIMATIONS, such as the Hartree-Fock method, ARE USUALLY INADEQUATE

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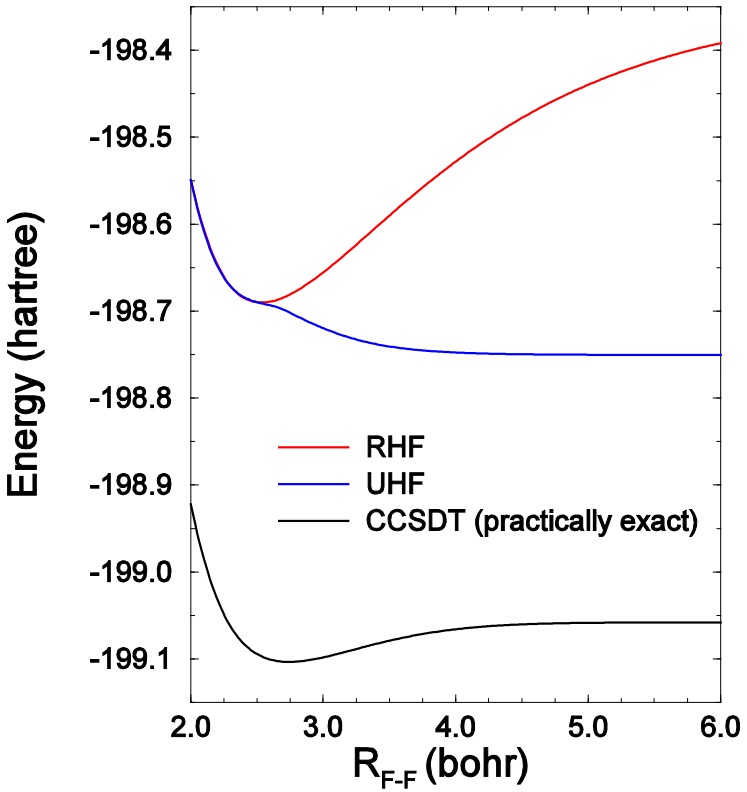
ELECTRONIC STRUCTURE:

Bond breaking in F_2



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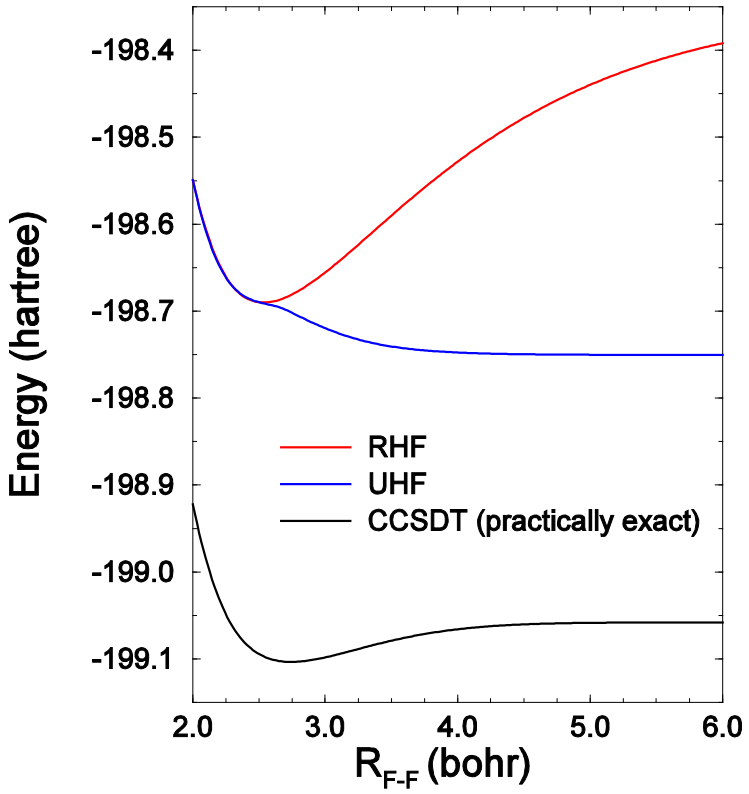

NUCLEAR STRUCTURE:

Binding energy of ^{4}He (4 shells)

Method	Energy (MeV)
$\langle \Phi_{osc} \vert H' \vert \Phi_{osc} \rangle$	-7.211
$\langle \Phi_{HF} \vert H' \vert \Phi_{HF} \rangle$	-10.520
CCSD	-21.978
CR-CCSD(T)	-23.524
Full Shell Model (Full CI)	-23.484

DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

This is a short course on single-reference MBPT aimed at the following content:

1. Preliminaries: molecular electronic Schrödinger equation, Slater determinants, CI wave function expansions, and elements of second quantization.
2. Rayleigh-Schrödinger perturbation theory, wave, reaction, and reduced resolvent operators.
3. Eigenfunction and eigenvalue expansions, renormalization terms, and bracketing technique.
4. Diagrammatic representation, rules for MBPT diagrams.
5. MBPT diagrams in low orders (second-, third-, and fourth-order energy corrections; first- and second-order wave function contributions).
6. Linked, unlinked, connected, and disconnected diagrams; diagram cancellations in fourth-order energy and third-order wave function corrections.
7. Linked and connected cluster theorem and their implications.

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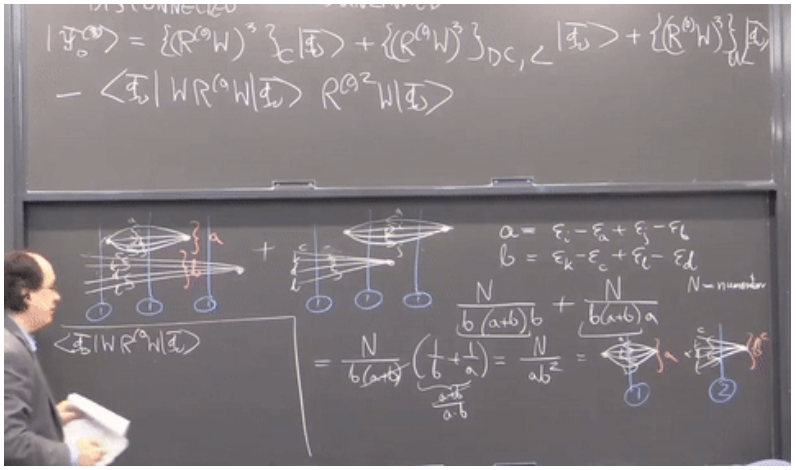
Time permitting, we will expand on point 7 and discuss basic elements of the coupled-cluster theory.

DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

This will be a short course on single-reference MBPT based on the following materials:

1. Lecture notes that will be provided to you in a PDF format.

2. The online lecture series entitled "Algebraic and Diagrammatic Methods for Many-Fermion Systems," available at
https://pages.wustl.edu/ppiecuch/course-videos
and on YouTube at
https://www.youtube.com/results?search_query=Chem+580&sp=CAI%253D,
recorded during my visit at Washington University in St. Louis in 2016, consisting of 44 videos (MBPT starts in lecture 28, with introductory remarks at the end of lecture 27).



3. Lecture notes by Professor Josef Paldus, which can be downloaded from www.math.uwaterloo.ca/~paldus/resources.html.

DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

Although the use of perturbation theory to analyze the many-electron correlation problem dates back to the seminal 1934 work by Møller and Plesset, the Møller and Plesset work is limited to the second order and does not use second quantization.

OCTOBER 1, 1934 PHYSICAL REVIEW VOLUME 46

Note on an Approximation Treatment for Many-Electron Systems

CHR. MØLLER AND M. S. PLESSET,* *Institut for teoretisk Fysik, Copenhagen*

(Received July 14, 1934)

A perturbation theory is developed for treating a system of n electrons in which the Hartree-Fock solution appears as the zero-order approximation. It is shown by this development that the first order correction for the energy and the charge density of the system is zero. The expression for the second-order correction for the energy greatly simplifies because of the special property of the zero-order solution. It is pointed out that the development of the higher approximation involves only calculations based on a definite one-body problem.

THE Hartree-Fock method[1] for treating a system of n electrons in a given external field consists in making the approximation of assigning to the system a wave function of the determinantal form

$$\Psi^0=\frac{1}{(n!)^{\frac{1}{2}}}\begin{vmatrix}\varphi_1(q_1) & \varphi_1(q_2) & \cdots & \varphi_1(q_n)\\ \varphi_2(q_1) & \cdot & \cdots & \cdot\\ \cdot & & & \cdot\\ \cdot & & & \cdot\\ \varphi_n(q_1) & \cdot & \cdots & \varphi_n(q_n)\end{vmatrix}, \quad (1)$$

where the variables q_i represent space and spin coordinates, and the n functions $\varphi_r(q)$ are a set of orthogonal normalized solutions of the equation

$$ih(\partial/\partial t)\varphi_r(q)=(H_0+B-A)\varphi_r(q). \quad (2)$$

In (2) H_0 is the Hamiltonian for an electron in the external field, and the matrix elements of B and A in the q-representation are given by[2]

$$(q|B|q')=\int\int(qq''|V|q'q''')dq''dq'''(q'''|\rho|q''), \quad (3)$$

$$(q|A|q')=\int\int(qq''|V|q'''q')dq''dq'''(q'''|\rho|q''), \quad (4)$$

where the matrix of ρ is defined by

$$(q|\rho|q')=\sum_{r=1}^{n}\varphi_r(q)\varphi_r^*(q'), \quad (5)$$

and V is the interaction energy for a pair of electrons.

As follows from the definition (5) the density matrix ρ is Hermitean and obeys the equation $\rho^2=\rho$; (5) together with (2) give the equation of motion for ρ

$$ih\dot{\rho}=(H_0+B-A)\rho-\rho(H_0+B-A). \quad (6)$$

As Dirac has emphasized, all probabilities can be expressed by means of this density matrix ρ;[3] in particular the charge density at q is given by $(q|\rho|q)$.

It is supposed throughout the following that H_0 does not contain the time explicitly. We may then consider solutions of (2) and (6) which belong to a stationary state μ so that our equations become

$$F_\mu\varphi_r^{(\mu)}(q)\equiv(H_0+B_\mu-A_\mu)\varphi_r^{(\mu)}(q)=\lambda_r^{(\mu)}\varphi_r^{(\mu)}(q); \quad (7)$$

$$F_\mu\rho_\mu-\rho_\mu F_\mu=0. \quad (8)$$

It is clear that the form of the operator F_μ depends on the stationary state considered. The energy of the system is, in the present approximation, given by

$$W_\mu^0=D\{\rho(H_0+\tfrac{1}{2}B_\mu-\tfrac{1}{2}A_\mu)\}, \quad (9)$$

where D denotes the diagonal sum. The corresponding wave function for a stationary state of the whole system is an eigenfunction of the operator

$$U_\mu\equiv\sum_{i=1}^{n}\{H_0^{(i)}+B_\mu^{(i)}-A_\mu^{(i)}\}=\sum_{i=1}^{n}F_\mu^{(i)}, \quad (10)$$

* National Research Fellow.

[1] V. Fock, Zeits. f. Physik **61**, 126 (1930); P. A. M. Dirac, Proc. Camb. Phil. Soc. **26**, Part III, 376 (1930).

[2] $\int\cdots dq$ is always understood to include summation over the spin coordinate.

[3] Dirac, Proc. Camb. Phil. Soc. **27**, Part II, 240 (1930).

DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

They key original papers most relevant to this presentation of MBPT are:

after these corrections and that for compound nucleus contribution a similar discrepancy yet remains, it is in the sense to correspond to a greater reduced width for neutrons (in C^{13}) than for protons (in N^{13}); i.e., "the neutrons stick out further than the protons." Such an effect has been suggested for heavier nuclei, though it would be very surprising to find it holding for so light a nucleus as $A=13$.

An estimate of the course of the cross section for the reaction $C^{12}(d,t)C^{11}$ was made on the basis of compound nucleus formation by assuming, as before, that the whole of the cross section for $C^{12}(d,n)N^{13}$ at low deuteron energies involves compound nucleus formation. On the assumption that the reduced width for triton emission is as great as that for neutron emission (the assumption of "preformed" tritons), we predict the dashed line of Fig. 2—in which the coming into play of successive residual states of C^{11} has been allowed for and the associated irregularities smoothed out. It is seen that even under the very unplausible assumption of the existence of preformed tritons, compound nucleus theory fails by an order of magnitude to explain the observed C^{11} formation. We are forced then to assume that this (d,t) reaction proceeds by some pickup mechanism and that we are indeed measuring the relative probability of the deuteron's losing a nucleon to the nucleus and removing one from it. As yet no sufficiently reliable theory of (d,t) pickup exists to warrant a comparison being made with these results. It is interesting to note that, at $E_d=3.3$ Mev, the angular distribution of the reaction $C^{13}(d,t)C^{12}$ is such as to suggest that a direct mechanism already predominates.[4]

It is interesting to compare these results with those of Cohen and Handley[9] on (p,t) reactions. These authors suggest that triton emission from a compound nucleus state has an inherent probability comparable with that for single nucleon emission. They base this argument on the rather flat angular distributions sometimes obtained which, they remark, tell against a pickup process. However, this conclusion is no longer valid when the energy of one or both the charged particles concerned is of the order of or below the Coulomb barrier; here a direct mechanism can give a sensibly isotropic angular distribution. It appears that considerable interest attaches to the resolution of this question of the mechanism by which tritons and similar complicated particles are emitted from nuclei in events of moderate to high energy.

[9] B. L. Cohen and T. H. Handley, Phys. Rev. **93**, 514 (1954)

PHYSICAL REVIEW VOLUME 100, NUMBER 1 OCTOBER 1, 1955

Many-Body Problem for Strongly Interacting Particles. II. Linked Cluster Expansion*

K. A. Brueckner
Indiana University, Bloomington, Indiana
(Received April 28, 1955)

An approximation method developed previously to deal with many particles in strong interaction is examined in further detail. It is shown that the series giving the interaction energy is a development in a sequence of linked or irreducible cluster terms each of which gives a contribution to the energy proportional to the total number of particles. Consequently the convergence of the expansion is independent of the total number of particles. The origin of this simple feature is illustrated by showing that a similar situation exists in the expansion of standard perturbation theory. The numerical convergence of the expansion is quantitatively discussed for the nuclear problem where it is shown that the correction arising from the first cluster term involving three particles is less than the leading term by a factor of about 10^{-4}. The smallness of the correction is largely a result of the action of the exclusion principle.

I. INTRODUCTION

IN a previous paper[1] (to be referred to as I) we have given a method for reducing approximately the many body problem for strongly interacting particles to a problem of self-consistent fields. Some of the physical content and origin of the method were discussed there and the nature of certain correction terms which can be neglected for very many particles was discussed. We shall in this paper examine the structure of another type of correction term which arises from interaction of clusters of particles and in so doing exhibit the general structure of the expansion involved. This will also allow us to draw some general conclusions about the convergence and accuracy of the method.

In Sec. II, we shall briefly summarize the relevant formulas from I and describe some difficulties which appear in high-order terms in the expansion for the energy which can be removed by a simple modification of the many-body propagation function. In Sec. III, we show how similar terms appear to arise in the usual perturbation theory but that they cancel identically, in a manner simply related to the cancellation discussed in Sec. II. In Sec. IV, we summarize these results and show how they may be generalized into a simple pre-

* Supported in part by a grant from the National Science Foundation.
[1] K. A. Brueckner and C. A. Levinson, Phys. Rev. **97**, 1344 (1955).

DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

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* Supported in part
Foundation.
[1] K. A. Brueckner an
(1955).

Derivation of the Brueckner many-body theory

By J. Goldstone

Trinity College, University of Cambridge‡

(*Communicated by N. F. Mott, F.R.S.—Received* 24 *August* 1956)

An exact formal solution is obtained to the problem of a system of fermions in interaction. This solution is expressed in a form which avoids the problem of unlinked clusters in many-body theory. The technique of Feynman graphs is used to derive the series and to define linked terms. The graphs are those appropriate to a system of many fermions and are used to give a new derivation of the Hartree–Fock and Brueckner methods for this problem.

1. Introduction

The Hartree–Fock approximation for the many-body problem uses a wave function which is a determinant of single-particle wave functions—that is, an independent-particle model. The single-particle states are eigenstates of a particle in a potential V, which is determined from the two-body interaction v by a self-consistent calculation. The Brueckner theory (Brueckner & Levinson 1955; Bethe 1956; Eden 1956) gives an improved method of defining V and shows why the residual effects of v not allowed for by V can be small. In particular, in the nuclear problem the corrections to the energy are small, even though the corrections to the wave function are large. The theory thus gives a reconciliation of the shell model, the strong two-nucleon interactions, and the observed two-body correlations in the nucleus. The smallness of the corrections is due to the operation of the exclusion principle. Bethe (1956) has shown that this same exclusion effect makes even the Hartree–Fock approximation good for quite strong interactions, such as an exponential potential fitted to low-energy nucleon-nucleon scattering.

The first problem on which calculations have been made is that of 'nuclear matter', that is, a very large nucleus with surface effects neglected (Brueckner 1955*a*; Wada & Brueckner 1956). In this problem the aim is to show that at a fixed density the energy is proportional to the number of particles, and that as the density is varied the energy per particle has a minimum at the observed density of large nuclei, and that this minimum value gives the observed volume energy of large nuclei. The single-particle wave functions are plane waves, and the potential V is diagonal in momentum space (in contrast to the ordinary Hartree potential which is diagonal in configuration space). The independent-particle model state is a 'Fermi gas' state with all the one-particle states filled up to the Fermi momentum k_F which depends only on the density.

Brueckner & Levinson's derivation, and that of Eden, is based on the multiple scattering formalism of Watson (Watson 1953). The proportionality of the energy of nuclear matter of a given density to the number of particles follows at once from the theory provided certain terms which represent several interactions occurring

‡ Author's present address: Institut for Teoretisk Fysik, Blegdamevej 17, Copenhagen.

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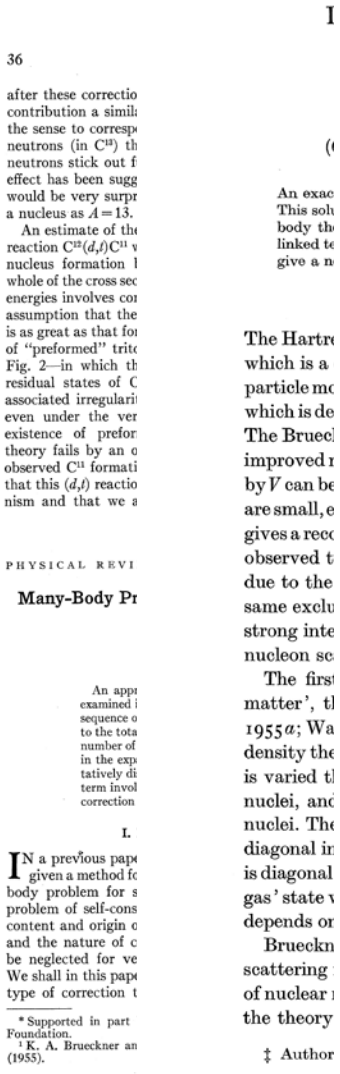

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The description of collective motions in terms of many-body perturbation theory

By J. Hubbard

Atomic Energy Research Establishment, Harwell, Didcot, Berkshire

(*Communicated by R. E. Peierls, F.R.S.—Received 2 February* 1957)

In this and a succeeding paper it is shown how a theory equivalent to the Bohm & Pines collective motion theory of the electron plasma can be derived directly from a perturbation series which gives in principle an exact solution of the many-body problem. This result is attained by making use of a diagrammatic method of analysis of the perturbation series. By a process analogous to the elimination of photon self-energy parts from the electrodynamic S matrix it is found possible to simplify the perturbation series, introducing a modified interaction between the particles. A useful integral equation for this modified interaction can be set up, and it is shown how the energy of the system can be expressed in terms of the modified interaction. The close connexion between this approach and the dielectric theory of plasma oscillations is indicated.

1. Introduction

Within recent years much attention has been given in the study of the quantum mechanical many-body problem to the collective modes of motion which may be present (Bohm & Pines 1953; Tomonaga 1955; Bohr & Mottelson 1953). Two main theories of collective motion have been developed, that of Tomonaga (1955), and the superfluous co-ordinate type of theory introduced by Bohm & Pines (1953). In the Tomonaga theory a transformation of variables is made in such a way that some of the new co-ordinates are directly related to the collective modes of motion, whilst the remaining new co-ordinates are associated with internal modes of motion. In the superfluous co-ordinate treatment certain auxiliary variables are introduced together with an equal number of subsidiary conditions to preserve the correct number of degrees of freedom, and a transformation is made in such a way that the new auxiliary variables are related to the collective motion, whilst the original co-ordinates when transformed are related to the internal motion. If the collective modes being studied have real physical significance, then it will be found in both these methods that the Hamiltonian is, to a good approximation, separable in the new co-ordinates, and a separation of the collective motion is thereby obtained.

Though these methods are quite successful, they have certain unsatisfactory features. In the Tomonaga method it is generally found that when the Hamiltonian has been separated the problem of finding the eigenvalues of the internal motion part is very difficult. In the superfluous co-ordinate treatment one does not meet with this difficulty but with an equivalent one; this is that it is difficult to find eigenfunctions satisfying the subsidiary conditions. In addition, both theories suffer from the difficulty of not being able to treat very easily the interaction between the collective and internal modes of motion, or the intimately related problem of the damping of the collective motion; where the damping is small this is not a very

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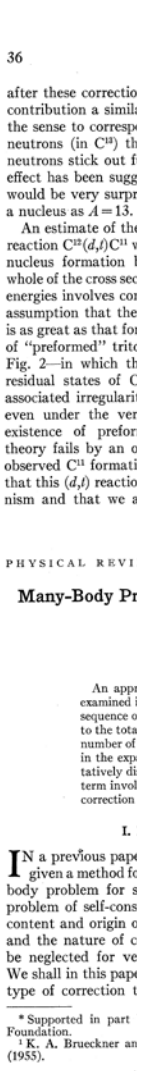

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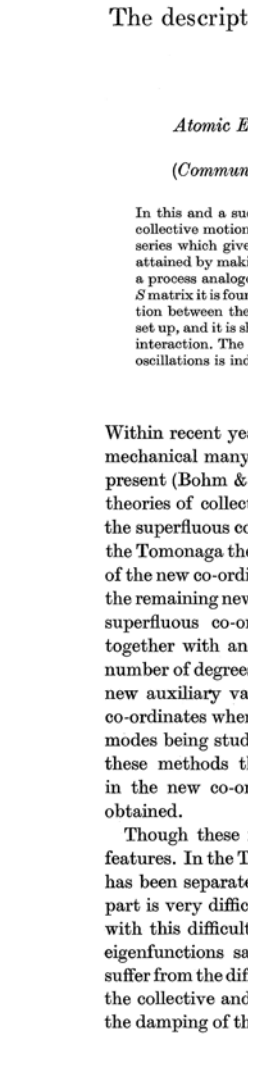

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PERTURBATION THEORY
OF LARGE QUANTUM SYSTEMS

by N. M. HUGENHOLTZ

Instituut voor theoretische fysica der Rijksuniversiteit, Utrecht, Nederland

Synopsis

The time-independent perturbation theory of quantum mechanics is studied for the case of very large systems, *i.e.* systems with large spatial dimensions (large volume Ω), and a large number of degrees of freedom. Examples of such systems are met with in the quantum theory of fields, solid state physics, the theory of imperfect gases and in the theory of nuclear matter. Only systems at or near the ground state (*i.e.*, systems at zero temperature) are treated in this paper. In the application of the conventional perturbation theory to such large quantum systems one encounters difficulties which are connected with the fact that even small perturbations produce large changes of the energy and wave function of the whole system. These difficulties manifest themselves through the occurrence of terms containing arbitrarily high powers of the volume Ω in the perturbation expansion of physical quantities. An extremely bad convergence of the perturbation expansion is the result.

For the analysis of the Ω-dependence of the terms in the expansion a new formulation of the time-independent perturbation theory is used, which was introduced by Van Hove. Making extensive use of diagrams to represent the different contributions to matrix elements it is possible to locate and separate the Ω-dependent terms, and to carry out partial summations in the original expansion. These separations and summations solve the above difficulties completely. Improved perturbation theoretical expressions are obtained for energies and wave functions of stationary states, as well as for the life-times of metastable states. All terms in these expressions are, in the limit of large Ω, either independent of Ω or proportional to Ω, corresponding to intensive or extensive physical quantities. The convergence of the improved perturbation expansions is no longer affected by the large magnitude of Ω.

CHAPTER I. INTRODUCTION

1. *The problem.* This paper is devoted to the perturbation theory of large quantum systems *i.e.*, quantum systems which have large spatial dimensions and a large number of degrees of freedom. The systems met with in the quantum theory of fields are, as is well known, of this type. Also in other branches of physics, such as quantum statistics and the Fermi gas model of heavy nuclei, one has to deal with such large systems. We shall in this paper only be interested in systems at or near the ground state. Our results are, therefore, only applicable to quantum systems at zero temperature.

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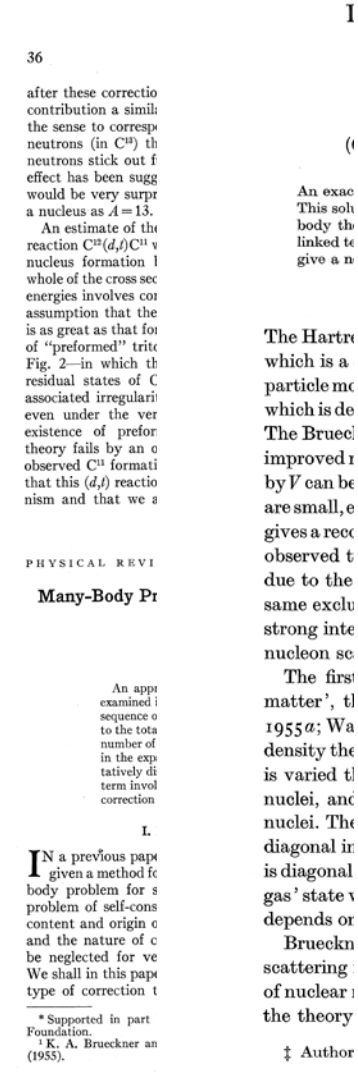

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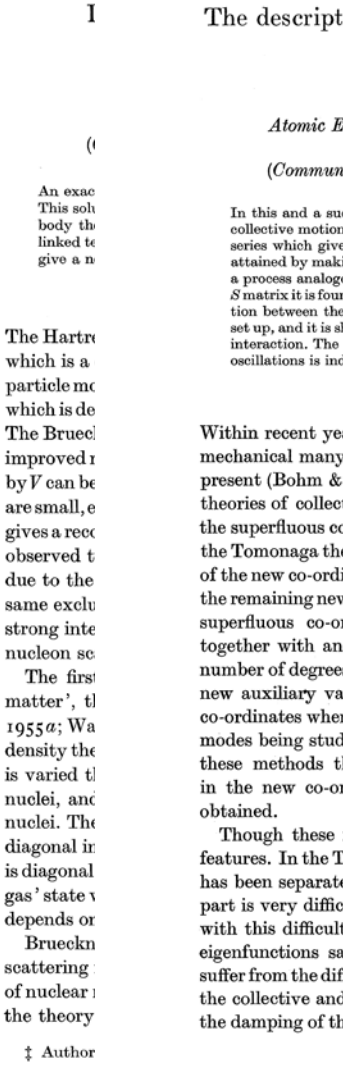

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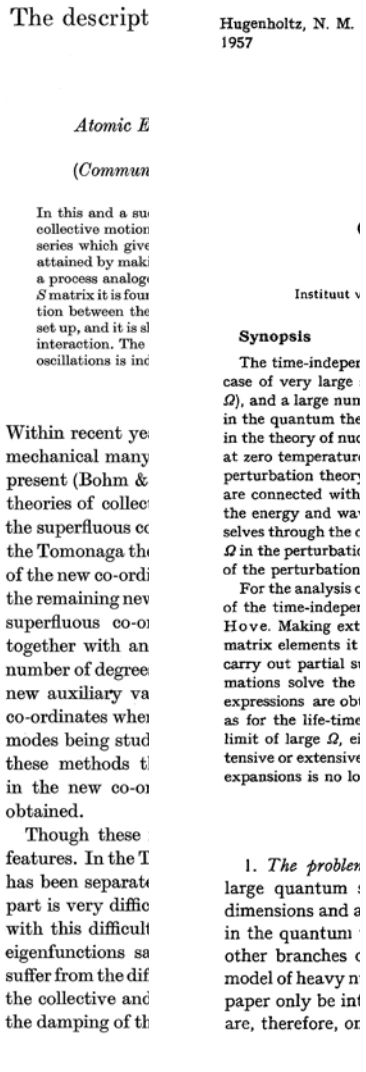

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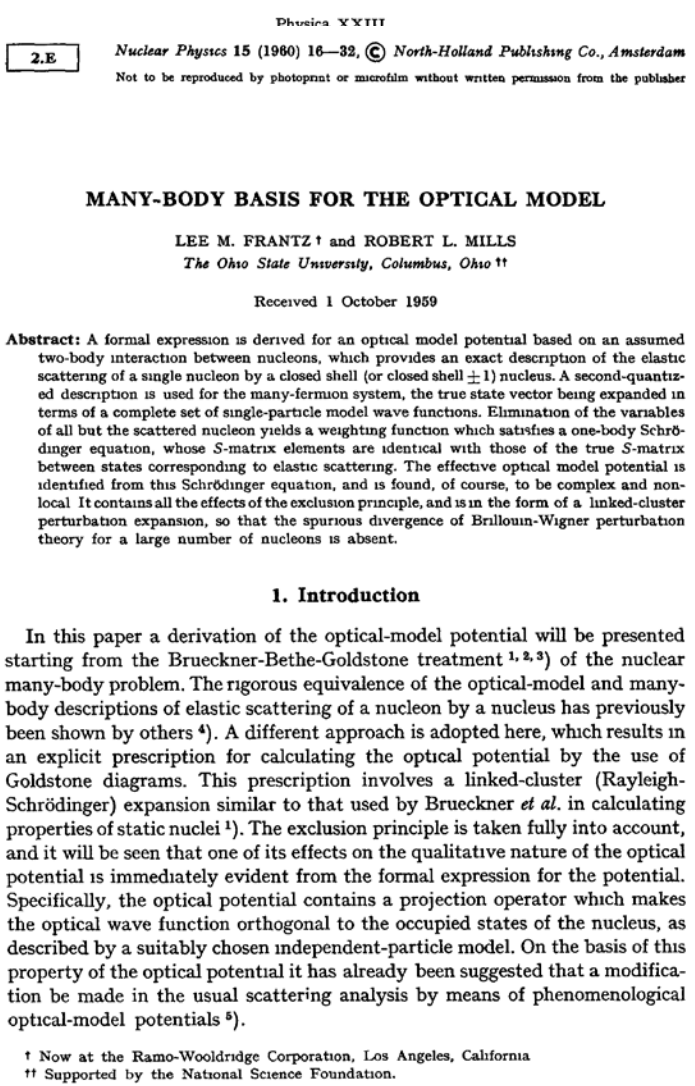

Physica XXIII

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Nuclear Physics 15 (1960) 16—32, © *North-Holland Publishing Co., Amsterdam*

MANY-BODY BASIS FOR THE OPTICAL MODEL

LEE M. FRANTZ † and ROBERT L. MILLS
The Ohio State University, Columbus, Ohio ††

Received 1 October 1959

Abstract: A formal expression is derived for an optical model potential based on an assumed two-body interaction between nucleons, which provides an exact description of the elastic scattering of a single nucleon by a closed shell (or closed shell ± 1) nucleus. A second-quantized description is used for the many-fermion system, the true state vector being expanded in terms of a complete set of single-particle model wave functions. Elimination of the variables of all but the scattered nucleon yields a weighting function which satisfies a one-body Schrödinger equation, whose S-matrix elements are identical with those of the true S-matrix between states corresponding to elastic scattering. The effective optical model potential is identified from this Schrödinger equation, and is found, of course, to be complex and non-local. It contains all the effects of the exclusion principle, and is in the form of a linked-cluster perturbation expansion, so that the spurious divergence of Brillouin-Wigner perturbation theory for a large number of nucleons is absent.

1. Introduction

In this paper a derivation of the optical-model potential will be presented starting from the Brueckner-Bethe-Goldstone treatment [1, 2, 3]) of the nuclear many-body problem. The rigorous equivalence of the optical-model and many-body descriptions of elastic scattering of a nucleon by a nucleus has previously been shown by others [4]). A different approach is adopted here, which results in an explicit prescription for calculating the optical potential by the use of Goldstone diagrams. This prescription involves a linked-cluster (Rayleigh-Schrödinger) expansion similar to that used by Brueckner *et al.* in calculating properties of static nuclei [1]). The exclusion principle is taken fully into account, and it will be seen that one of its effects on the qualitative nature of the optical potential is immediately evident from the formal expression for the potential. Specifically, the optical potential contains a projection operator which makes the optical wave function orthogonal to the occupied states of the nucleus, as described by a suitably chosen independent-particle model. On the basis of this property of the optical potential it has already been suggested that a modification be made in the usual scattering analysis by means of phenomenological optical-model potentials [5]).

† Now at the Ramo-Wooldridge Corporation, Los Angeles, California
†† Supported by the National Science Foundation.

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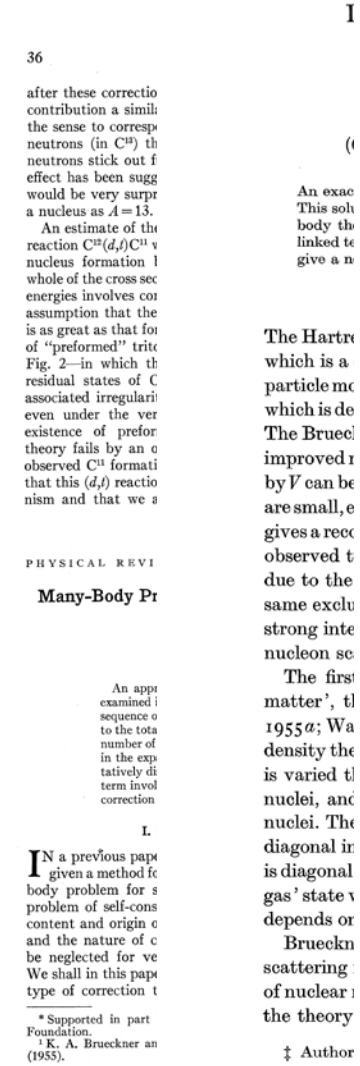

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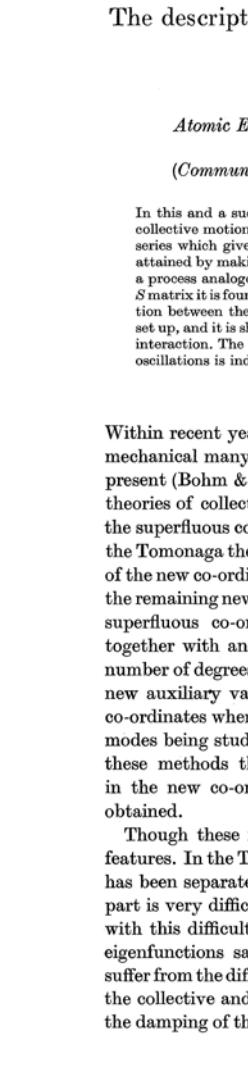

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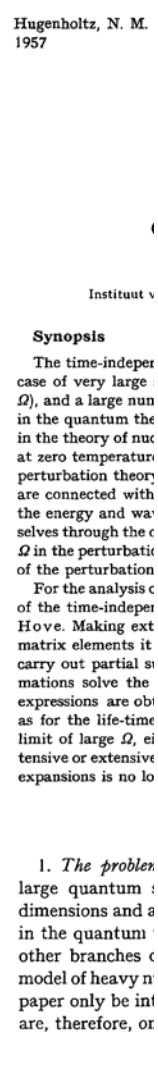

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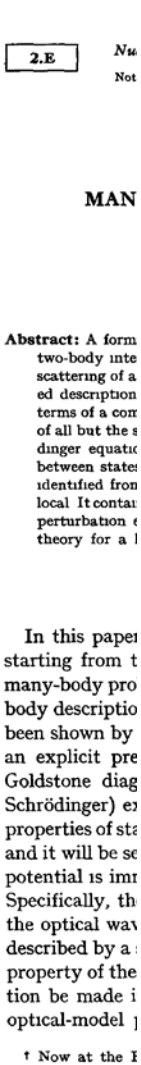

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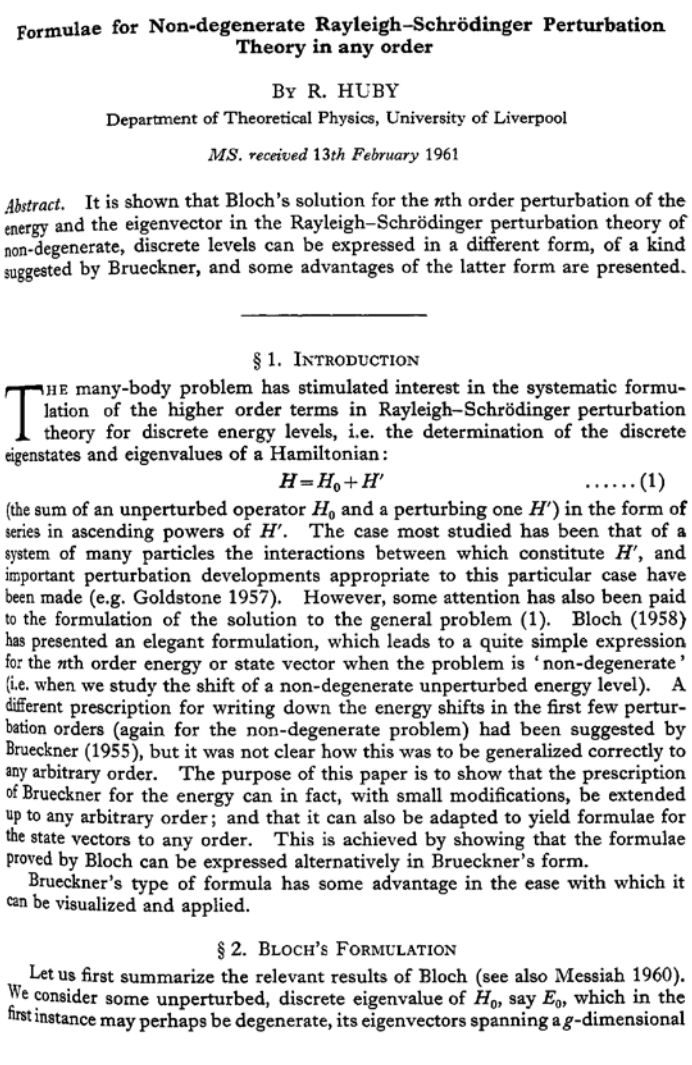

Formulae for Non-degenerate Rayleigh–Schrödinger Perturbation Theory in any order

BY R. HUBY

Department of Theoretical Physics, University of Liverpool

MS. received 13*th February* 1961

Abstract. It is shown that Bloch's solution for the nth order perturbation of the energy and the eigenvector in the Rayleigh–Schrödinger perturbation theory of non-degenerate, discrete levels can be expressed in a different form, of a kind suggested by Brueckner, and some advantages of the latter form are presented.

§ 1. INTRODUCTION

THE many-body problem has stimulated interest in the systematic formulation of the higher order terms in Rayleigh–Schrödinger perturbation theory for discrete energy levels, i.e. the determination of the discrete eigenstates and eigenvalues of a Hamiltonian:

$$H = H_0 + H' \qquad \ldots\ldots(1)$$

(the sum of an unperturbed operator H_0 and a perturbing one H') in the form of series in ascending powers of H'. The case most studied has been that of a system of many particles the interactions between which constitute H', and important perturbation developments appropriate to this particular case have been made (e.g. Goldstone 1957). However, some attention has also been paid to the formulation of the solution to the general problem (1). Bloch (1958) has presented an elegant formulation, which leads to a quite simple expression for the nth order energy or state vector when the problem is 'non-degenerate' (i.e. when we study the shift of a non-degenerate unperturbed energy level). A different prescription for writing down the energy shifts in the first few perturbation orders (again for the non-degenerate problem) had been suggested by Brueckner (1955), but it was not clear how this was to be generalized correctly to any arbitrary order. The purpose of this paper is to show that the prescription of Brueckner for the energy can in fact, with small modifications, be extended up to any arbitrary order; and that it can also be adapted to yield formulae for the state vectors to any order. This is achieved by showing that the formulae proved by Bloch can be expressed alternatively in Brueckner's form.

Brueckner's type of formula has some advantage in the ease with which it can be visualized and applied.

§ 2. BLOCH'S FORMULATION

Let us first summarize the relevant results of Bloch (see also Messiah 1960). We consider some unperturbed, discrete eigenvalue of H_0, say E_0, which in the first instance may perhaps be degenerate, its eigenvectors spanning a g-dimensional

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DESCRIPTION OF MANY-PARTICLE CORRELATION EFFECTS BY SINGLE-REFERENCE MANY-BODY PERTURBATION THEORY (MBPT)

They key original papers most relevant to this presentation of MBPT are:

- K. A. Brueckner, *Phys. Rev.* **100**, 36 (1955).
- J. Goldstone, *Proc. R. Soc. Lond., Ser A* **239**, 267 (1957).
- J. Hubbard, *Proc. R. Soc. Lond., Ser. A* **240**, 539 (1957).
- N. M. Hugenholtz, *Physica* **23**, 481 (1957).
- L. M. Frantz and R. L. Mills, *Nucl. Phys.* **15**, 16 (1960).
- R. Huby, *Proc. Phys. Soc*. **78**, 529 (1961).

The discussion of the Rayleigh-Schrödinger perturbation theory and reduced resolvents, especially in the video lecture series, is taken from P. O. Löwdin, in Perturbation Theory and Its Applications in Quantum Mechanics, edited by C. H. Wilcox (John Wiley & Sons, New York, 1966), pp. 255-294, and references therein.

KEY THEOREMS OF MBPT

Linked cluster (diagram) theorem (Brueckner, 1955; Goldstone, 1957)

MBPT

$$\begin{aligned} \Psi^{(k)} &= (R_0 W)^k \Phi_0 + \text{renormalization terms} \\ &= \left[(R_0 W)^k\right]_{\text{linked}} \Phi_0 \,, \quad (k = 1, 2, \ldots), \end{aligned}$$

$$\begin{aligned} \Delta E^{(k+1)} &= \langle \Phi_0 | W (R_0 W)^k | \Phi_0 \rangle + \text{renormalization terms} \\ &= \langle \Phi_0 | \left[W (R_0 W)^k\right]_{\text{connected}} | \Phi_0 \rangle \,, \quad (k = 1, 2, \ldots). \end{aligned}$$

Connected cluster theorem (Hubbard, 1957; Hugenholtz, 1957)

$$\Psi = e^T \Phi, \quad T = \sum_{k=1}^{\infty} \sum_C \{(R_0 W)^k\}_C$$

$$C \Leftrightarrow \text{connected diagrams (including EPV terms)}$$

- **Finite-order MBPT calculations lead to a size extensive description of many-fermion systems, so that no loss of accuracy occurs when the system is made larger.**
- **One can generate the entire infinite-order MBPT series via the exponential wave function ansatz of coupled-cluster theory, which is size extensive and which can be made size consistent if the reference determinant is separable.**

Although the initial proposals suggesting the use of the exponential wave function ansatz of coupled-cluster theory in the context of the many-fermion correlation problem (especially, in nuclei) date back to 1958 and 1960,

1.C *Nuclear Physics* 7 (1958) 421—424; © *North-Holland Publishing Co., Amsterdam*

BOUND STATES OF A MANY-PARTICLE SYSTEM

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Received 10 April 1958

Abstract: Rigorous formal solutions of the bound state Schrödinger equation are constructed in terms of an arbitrary complete set of single particle wave functions. From these solutions one sees without effort that the Rayleigh Schrödinger perturbation expansion of the energy does not contain matrix elements represented by products of unlinked diagrams. The components of the state vector are related in a simple manner to functions represented by linked diagrams only.

The validity of the Brueckner approximation to the bound state energy of a many particle system depends on the absence of "unlinked clusters" in the perturbation expansion of this energy. Brueckner [1]) has shown that such terms are absent from a few orders of the perturbation series. General proofs for all orders of the perturbation series have been given by several authors [2–4]). All these proofs are based on a detailed inspection of perturbation terms of arbitrary order. The purpose of this note is to cast the basic equations into such a form that the absence of unlinked terms from the energy becomes evident without detailed inspection of all n'th order perturbation matrix elements.

We are concerned with the formal perturbation expansion of the bound state Ω of a many particle system in terms of the eigenstates of a suitable independent particle Hamiltonian H_0. The expansion in powers of the perturbation $W \equiv H - H_0$ need not converge. However, if the interaction potential is bounded, the perturbation expansion of the state Ω_η,

$$(H_0+\eta W)\Omega_\eta = E_\eta \Omega_\eta \qquad (1)$$

converges for sufficiently small η, $0 < \eta \leqq 1$. There is an unambiguous correspondence between Ω_η and the zero order eigenstate ϕ defined by † $\phi = \lim_{\eta=0} \Omega_\eta$,

$$H_0\phi = E_0\phi.$$

The formal properties of the terms in the perturbation series are the same for all values of η. After a suitable selective summation of the leading terms in the series [2]) the limit $\eta \to 1$ may exist even if it did not exist for the original series. The correspondence $\phi \longleftrightarrow \Omega$ persists. ϕ is the "model state" of Eden and Francis [6]) and the "chosen configuration" of Bethe [7]). For an

† For proof of these statements see for instance F. Riesz and B. Sz. Nagy, ref. [5]).

1.C: 1.D.1 *Nuclear Physics* **17** (1960) 477—485; © *North-Holland Publishing Co., Amsterdam*

SHORT-RANGE CORRELATIONS IN NUCLEAR WAVE FUNCTIONS

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Received 18 February 1960

Abstract: We assume that the ground state wave functions of a closed shell nucleus is approximated by a Slater determinant in the restricted region of configuration space where all internucleon distances are larger than a certain "healing distance". The remainder of the wave function is given in terms of a series of cluster functions. The overlap integral between the correct wave functions and the Slater determinant is small and depends on the higher cluster functions in a complicated manner. Nevertheless we can show that the one- and two-body density matrices are well approximated by expressions involving only the single-particle wave functions and the two-body cluster functions. The Schrödinger equation yields a coupled set of equations which determine the cluster functions as well as the single-particle wave functions.

1. Introduction

In any attempt to relate the nuclear shell model to the many-body problem with two-body forces the question arises whether the shell-model state Φ approximates the correct state vector Ψ in some sense or whether there is merely a certain correspondence [1]) between them. The overlap integral between the two wave functions is known to be small for large nuclei [2–4]). On the other hand there are good reasons to believe that the two functions approximate each other if all particles are sufficiently separated [5]). It is the purpose of this note to exploit the mathematical consequences of such a relation, and discuss a formalism which allows us to calculate corrections to the shell model wave functions by perturbation theory for separated particles while using different approximations where two or several particles are close to each other. The results of such a procedure must, of course, be related to the well-known selective summations of the perturbation series [2, 6–10]). We restrict ourselves to ground states of closed shell nuclei where we expect no long range correlations in the wave functions and non-degenerate perturbation theory is applicable. In the middle of the shell one must account for the well known collective features of the wave function as well as for the short range correlations. This problem will be dealt with a later paper. Nuclear matter is not an idealization of a closed shell nucleus.

† Work supported in part by the U. S. Atomic Energy Commission.

the paper that led to the wide-spread use of coupled-cluster theory and its diagrammatic formulation, especially in the context of the many-electron correlation problem, is the 1966 article by J. Čížek:

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On the Correlation Problem in Atomic and Molecular Systems. Calculation of Wavefunction Components in Ursell-Type Expansion Using Quantum-Field Theoretical Methods

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(Received 17 May 1966)

A method is suggested for the calculation of the matrix elements of the logarithm of an operator which gives the exact wavefunction when operating on the wavefunction in the one-electron approximation. The method is based on the use of the creation and annihilation operators, hole-particle formalism, Wick's theorem, and the technique of Feynman-like diagrams. The connection of this method with the configuration-interaction method as well as with the perturbation theory in the quantum-field theoretical form is discussed. The method is applied to the simple models of nitrogen and benzene molecules. The results are compared with those obtained with the configuration-interaction method considering all possible configurations within the chosen basis of one-electron functions.

I. FORMULATION OF THE PROBLEM

LET us consider a system consisting of fixed atomic nuclei and $2n$ electrons. Let us further exclude from our considerations systems having a degenerate ground state. Then, neglecting relativistic and magnetic effects, the Hamiltonian $\hat{H}$ of our problem is given by the following equations:

$$\hat{H}=\hat{Z}+\hat{V}, \tag{1}$$

$$\hat{Z}=\sum_i \hat{z}_i, \qquad \hat{V}=\sum_{i<j} \hat{v}_{i,j}, \tag{2}$$

where $\hat{z}_i$ is a one-particle operator corresponding to the sum of the kinetic and nuclear field energy, and $\hat{v}_{i,j}$ is a two-particle operator of the interelectronic Coulombic repulsion.

Our problem is to find the ground-state eigenvector and the corresponding eigenvalue of the Hamiltonian (1)

$$\hat{H}\,|\Psi\rangle=E\,|\Psi\rangle. \tag{3}$$

In order to solve this problem the wavefunction $|\Psi\rangle$ is written in the following form

$$|\Psi\rangle=\exp(\hat{T})\,|\Phi\rangle, \tag{4}$$

where $|\Phi\rangle$ is the ground-state wavefunction in the one-particle approximation. This form of the wavefunction[1–5] is connected with the so-called Ursell-type expansion. The use of an expansion of this type for the study of the electronic structure of atoms and molecules was suggested by Sinanoğlu.[3]

In this article, equations for the matrix elements of the operator $\hat{T}$ are derived using quantum-field theoretical concepts, namely, (1) the creation and annihilation operators, (2) the hole–particle formalism, (3) the time-independent Wick theorem and the diagram technique.

In addition, the connection of the proposed method with both the configuration-interaction method and the perturbation theory in the quantum-field theoretical form[6,7] are shown. This comparison demonstrates the usefulness of the Ursell-type expansion of the exact wavefunction.

II. BASIC TERMS AND DEFINITIONS

Let us introduce a complete set of orthonormal spin-orbitals

$$|A\rangle=|a\rangle\,|\alpha\rangle, \tag{5}$$

where $|a\rangle$ and $|\alpha\rangle$ designate the space and the spin parts of the spin-orbital $|A\rangle$, respectively. Generally, capital letters are used to designate spin–orbitals, lower-case letters are associated with orbitals, while letters of the Greek alphabet are reserved for spin functions. In addition to this general system of spin–orbitals (5), we use spin–orbitals whose space parts are eigenfunctions of the operator

$$(\hat{z}+\hat{u})\,|a\rangle=\omega_a\,|a\rangle, \tag{6}$$

where $\hat{u}$ is an arbitrary spin-independent one-particle Hermitian operator. Let us note explicitly that Hartree–Fock spin–orbitals fall within this class.

The creation and annihilation operators defined on the system of spin-orbitals (5) are designated $\hat{X}_A^+$ and $\hat{X}_A$, respectively. These operators satisfy the following anticommutation relations:

$$\hat{X}_A^+\hat{X}_B^+ + \hat{X}_B^+\hat{X}_A^+ = 0,$$

$$\hat{X}_A\hat{X}_B + \hat{X}_B\hat{X}_A = 0,$$

$$\hat{X}_A\hat{X}_B^+ + \hat{X}_B^+\hat{X}_A = \langle A|B\rangle. \tag{7}$$

* Part of this study was carried out during the author's stay in the Centre de Mécanique Ondulatoire Appliquée, Paris, France.
[1] F. Coester and H. Kümmel, Nucl. Phys. **17**, 477 (1960).
[2] H. Kümmel, *Lectures on The Many-Body Problem*, E. R. Caianiello, Ed. (Academic Press Inc., New York, 1962), p. 265.
[3] O. Sinanoğlu, J. Chem. Phys. **36**, 706 (1962); Advan. Chem. Phys. **6**, 315 (1964).
[4] H. Primas, Lecture prepared for the Istanbul International Summer School of Quantum Chemistry, 1964 (preprint).
[5] J. da Providencia, Nucl. Phys. **61**, 87 (1965).
[6] J. Goldstone, Proc. Roy. Soc. (London) **239**, 267 (1957).
[7] V. V. Tolmachev, "The field form of the perturbation theory applied to many electron problems of atoms and molecules," University of Tartu, 1963 (in Russian).

If time permits, we will talk about it, at least a little, after discussing MBPT.

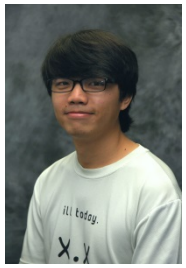
THANK YOU

Dr. Jun Shen (2010-present)

Emiliano Deustua (2014-present)

Ilias Magoulas (2015-present)

Stephen Yuwono (2017-present)



Arnab Chakraborty (2018-present)

"Algebraic and Diagrammatic Methods for Many-Fermion Systems"

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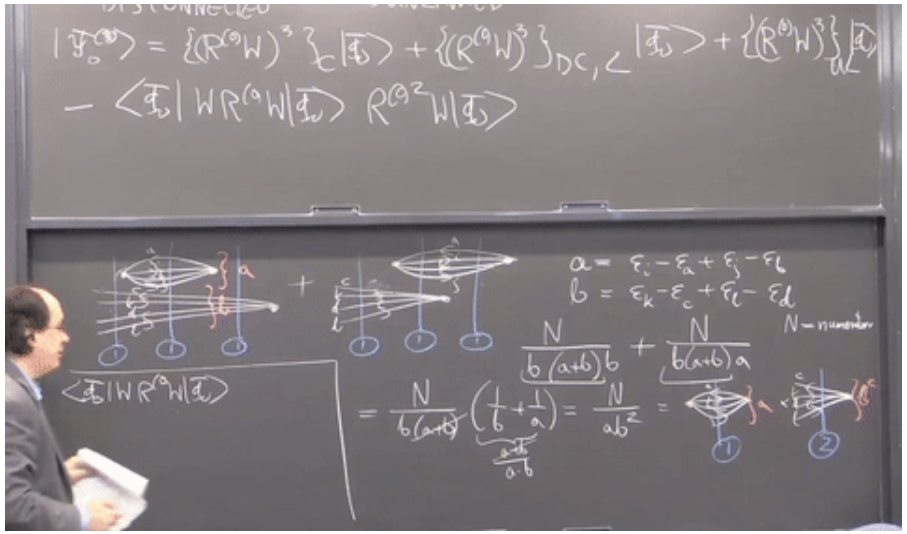

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