Title
ON THE CONNECTION OF THE INDEPENDENT-PAIR MODEL WITH A VARIATIONAL PRINCIPLE

Author
Dietrich, Klaus.

Publication Date
1963-11-19

UCRL-11123

University of California

Ernest O. Lawrence Radiation Laboratory

ON THE CONNECTION OF THE INDEPENDENT-PAIR MODEL WITH A VARIATIONAL PRINCIPLE

Berkeley, California

DISCLAIMER

Submitted for publication in
Zestschrift fur Physik

UCRL-11123

UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California

AEC Contract No. W-7405-eng-48

ON THE CONNECTION OF THE INDEPENDENT-PAIR MODEL WITH A VARIATIONAL PRINCIPLE

Klaus Dietrich

November 19, 1963

ON THE CONNECTION OF THE INDEPENDENT-PAIR MODEL WITH A VARIATIONAL PRINCIPLE*

Klaus Dietrich

Lawrence Radiation Laboratory
University of California
Berkeley, California

November 19, 1963

ABSTRACT

It is shown that Brenig's method of deriving the basic equations of the Independent-Pair Model can also be understood from a variational principle applied to the pseudo-expectation value $\langle \Pi | H | \Psi \rangle$ (Π = model wave function, Ψ = true wave function). Deviations from a vanishing first and second variation of $\langle \Pi | H | \Psi \rangle$ with respect to the model wave function Π are shown to be due only to the independent-pair approximation, and thus permit us to make a qualitative estimate of the accuracy of this method.

INTRODUCTION

The basic equations of the Independent-Pair Model have been derived in many different ways. The present work may be regarded as a corollary of the formulation given by Brenig.[1] It originates from the question of whether a solution of the basic equations of the model must always coincide with a stationary value of the "pseudo-expectation value" $\langle \Pi | H | \Psi \rangle$; Π being a model wave function defined in (1.1), and $\Psi(1 \ldots A)$ the true wave function of the A-body problem.

In one of the early papers on Brueckner's method, Eden gave a proof that a variation of $\langle \Pi | H | \Psi \rangle$ with respect to the one-particle functions in Π was equivalent to the one-particle equations of the model, up to terms of the order 1/A (A = number of particles).[2] Later Eden, Emery, and Sampanthar[3] performed calculations on O^{16}, Mang and Wild considered tritium and helium-4,[4] and the author treated helium-5 in the independent pair approximation.[5] The method was also applied to light hyperfragments.[6,7] In the case of the three-, four-, and five-body problems, the energy E, evaluated with the approximate solutions of the one- and two-particle equations, agreed quite well with a stationary value of $\langle \Pi | H | \Psi \rangle$, whereas the agreement was not so good in the case of O^{16}. If this discrepancy was due to terms of the order 1/A, as Eden's proof might suggest, one would expect the opposite trend.

In this paper, we want to show that except for errors inherent in the independent pair approximation, the one- and two-particle equations of the Independent-Pair Model are exactly equivalent to the requirement that the first and second variation of $\langle \Pi | H | \Psi \rangle$ with respect to Π should vanish.

1. Introduction to Brenig's Formalism

We define a set of A linearly independent single-particle functions $\varphi^{\lambda}(\lambda)$. One may think of them as the A lowest eigenfunctions corresponding to some single-particle model, and we shall sometimes refer to these functions as "model wave

function."

Throughout the paper, an argument $\lambda,\mu,\cdots$ will represent all the coordinates (space, spin, possibly isospin) of a particle, and an index $\lambda,\mu\cdots$ will define the quantum state.

We take $\Psi(1\cdots A)$ to be the true antisymmetric wave function of the A-particle system and introduce the following products of superscripted single-particle functions:

$$\Pi^{\prime}: = \prod_{\lambda=1}^{A} \varphi^{\lambda}(\lambda) \tag{1-1}$$

$$\Pi^{\mu}: = \prod_{\substack{\lambda=1 \\ \lambda\neq\mu}}^{A} \varphi^{\lambda}(\lambda) \tag{1-2}$$

$$\Pi^{\mu\nu}: = \prod_{\substack{\lambda=1 \\ \lambda\neq\mu,\nu}}^{A} \varphi^{\lambda}(\lambda) \tag{1-3}$$

Except where otherwise noted, all indices are restriced to $1,\cdots,A$. We can now define subscripted functions as projections of $\Psi(1\cdots A)$ on the product wave functions;

$$\varphi_{\mu}: = \langle \Pi^{\mu} | \Psi \rangle \tag{1-4}$$

$$\psi_{\mu\nu}: = \langle \Pi^{\mu\nu} | \Psi \rangle \tag{1-5}$$

$$\psi_{\mu\nu\kappa}: = \langle \Pi^{\mu\nu\kappa} | \Psi \rangle \tag{1-6}$$

The hexagonal bracket symbols indicate integration and summation over all coordinates appearing in the bra-states. If we have the same symbols in the same order for the arguments and the state numbers, we omit the arguments. We choose the normalization to be

$$\langle \Pi \mid \Psi \rangle = 1. \tag{1-7}$$

Of course, the superscripted single-particle functions must be chosen so that Π is not orthogonal to Ψ. It follows from these definitions that functions with more than one subscript are antisymmetric with respect to an interchange of any two arguments or any two subscripts:

$$\psi_{\mu\nu}(\mu\nu) = -\psi_{\mu\nu}(\nu\mu) = -\psi_{\nu\mu}(\mu\nu). \tag{1-8}$$

Furthermore, it can readily be shown that the following orthogonality relations hold:

$$\langle \varphi^{\mu} \mid \varphi_{\nu} \rangle = \delta_{\mu\nu}, \tag{1-9}$$

$$\langle \varphi^{\kappa} \mid \psi_{\mu\nu} \rangle = \delta_{\kappa\nu} \varphi_{\mu}(\mu) - \delta_{\kappa\mu} \varphi_{\nu}(\mu). \tag{1-10}$$

In these definitions the functions are defined only for indices smaller than or equal to A. The functions φ^{λ} and φ_{λ} may, however, be respectively extended to form a complete basis (see reference 1), with the condition (1-9) holding for all functions of the complete system.

The Hamiltonian for the A-body problem is

$$H = \sum_{\kappa} T(\kappa) + \frac{1}{2} \sum_{\kappa,\lambda} v(\kappa,\lambda), \tag{1-11}$$

and we can write the total energy E as

$$E = \langle \Pi | H | \Psi \rangle = \sum_{\kappa} \langle \varphi^{\kappa} | T | \varphi_{\kappa} \rangle + \frac{1}{2} \sum_{\kappa,\lambda} \langle \varphi^{\kappa} \varphi^{\lambda} | v | \psi_{\kappa\lambda} \rangle \quad (1\text{-}12)$$

where T is the kinetic energy operator and v the nucleon-nucleon potential. All the correlating functions vanish automatically if any two of their subscripts are equal and, therefore, we need not restrict the summations to unequal values of the indices.

Equation (1-12) is the starting point of our derivation.

2. Brenig's Method from the Standpoint of a Variational Principle.

We define a first variation of the product function as follows:

$$\delta_{\mu} \Pi = \delta \varphi^{\mu} \Pi^{\mu}. \quad (2\text{-}1)$$

The variation must not violate the normalization condition (1-7), i.e.,

$$\langle \delta_{\mu} \Pi \mid \Psi \rangle = \langle \delta \varphi^{\mu} \mid \varphi_{\mu} \rangle = 0. \quad (2\text{-}2)$$

We require that the first variation of $\langle \Pi | H | \Psi \rangle$ with respect to the model wave function Π should vanish. By the use of a Lagrange multiplier E we can vary Π without restrictions:

$$\langle \delta_{\mu} \Pi | H - E | \Psi \rangle = 0. \quad (2\text{-}3)$$

From (1-12) we have

$$\langle \delta \varphi^{\mu} | T | \varphi_{\mu} \rangle + \sum_{\rho} \langle \delta \varphi^{\mu} \varphi^{\rho} | v | \psi_{\mu\rho} \rangle + \sum_{\rho \neq \mu} \langle \varphi^{\rho} | T | \delta_{\mu} \varphi_{\rho} \rangle \quad (2\text{-}4)$$

$$+ \frac{1}{2} \sum_{\rho,\kappa \neq \mu} \langle \varphi^\rho \varphi^\kappa \,|v|\, \delta_\mu \psi_{\rho\kappa} \rangle - E \langle \delta\varphi^\mu | \varphi_\mu \rangle = 0.$$

and using

$$\delta_\mu \varphi_\rho = \langle \delta\varphi^\mu | \psi_{\mu\rho} \rangle \tag{2-5}$$

$$\delta_\mu \psi_{\rho\kappa}\,(\rho,\kappa)'' = \langle \delta\varphi^\mu \,|\, \psi_{\mu\rho\kappa} \rangle, \tag{2-6}$$

we obtain immediately

$$\langle \delta\varphi^\mu \,|T|\, \varphi_\mu \rangle + \sum_\rho \langle \delta\varphi^\mu \varphi^\rho \,|v|\, \psi_{\mu\rho} \rangle + \sum_\rho \langle \delta\varphi^\mu \varphi^\rho \,|T(\rho)|\, \psi_{\mu\rho} \rangle \tag{2-7}$$

$$+ \frac{1}{2} \sum_{\rho,\kappa} \langle \delta\varphi^\mu \varphi^\rho \varphi^\kappa |v(\rho,\kappa)| \psi_{\mu\rho\kappa} \rangle - E \langle \delta\varphi^\mu \,|\, \varphi_\mu \rangle = 0.$$

Since there are certainly variations $\delta\varphi^\mu$ for which the different integrals in (2-7) do not vanish automatically, Eq. (2-7) is equivalent to

$$T(\mu)\varphi_\mu + \sum_\rho \langle \varphi^\rho \,|v|\, \psi_{\mu\rho} \rangle + \sum_\rho \langle \varphi^\rho \,|T(\rho)|\, \psi_{\mu\rho} \rangle$$

$$+ \frac{1}{2} \sum_{\rho,\kappa} \langle \varphi^\rho \varphi^\kappa |v(\rho,\kappa)| \psi_{\mu\rho\kappa} \rangle = E \varphi_\mu. \tag{2-8}$$

We now define second variations of the product function Π by

$$\delta_{\mu\nu}\Pi := \delta\varphi^{\mu}\ \delta\varphi^{\nu}\ \Pi^{\mu\nu} . \tag{2-9}$$

We consider only the case $\mu \neq \nu$ in the following; the case $\mu = \nu$ is trivial and without interest. Again, the normalization condition should also hold for the varied function, i.e., we have to require that

$$\langle \delta_{\mu\nu}\Pi \,|\, \underline{\Psi}\rangle = \langle \delta\varphi^{\mu}\ \delta\varphi^{\nu}\,|\,\psi_{\mu\nu}\rangle = 0 . \tag{2-10}$$

Dealing with this restriction by a Lagrange multiplier E', we require the second variation of $\langle \Pi \,|\, H \,|\, \underline{\Psi}\rangle$ to vanish,

$$\langle \delta_{\mu\nu}\Pi \,|\, H\text{-}E' \,|\, \underline{\Psi}\rangle = 0 . \tag{2-11}$$

This leads immediately to

$$\begin{aligned}
&\langle \delta\varphi^{\mu}\ \delta\varphi^{\nu}|T(\mu)\ \ T(\nu)\ \ V(\mu\nu)|\psi_{\mu\nu}\rangle + \sum_{\rho}\langle \delta\varphi^{\mu}\ \delta\varphi^{\nu}\ \varphi^{\rho}|V(\mu.\rho) + V(\nu.\rho)|\psi_{\mu\lambda\rho}\rangle \\
&+ \sum_{\rho}\langle \delta\varphi^{\mu}\ \delta\varphi^{\nu}\ \varphi^{\rho}|T(\rho)|\psi_{\mu\nu\rho}\rangle + \frac{1}{2}\sum_{\kappa,\rho}\langle \delta\varphi^{\mu}\ \delta\varphi^{\nu}\varphi^{\rho}\ \varphi^{\kappa}|V(\rho\kappa)|\psi_{\mu\nu\rho\kappa}\rangle \\
&- E'\,\langle \delta\varphi^{\mu}\ \delta\varphi^{\nu}|\psi_{\mu\nu}\rangle = 0 ,
\end{aligned} \tag{2-12}$$

and this is equivalent to

$$\begin{aligned}
&[T(\mu) + T(\nu) + V(\mu\nu)]\ \ _{\mu\nu} + \sum_{\rho}\langle \varphi^{\rho}|V(\mu\rho) + V(\nu\ \rho)|\psi_{\mu\nu\rho}\rangle \\
&+ \sum_{\rho}\langle \varphi^{\rho}|T(\rho)|\ \psi_{\alpha\nu\rho}\rangle + \frac{1}{2}\sum_{\kappa\rho}\langle \varphi^{\rho}\ \varphi^{\kappa}|V(\rho\ \kappa)|\ \psi_{\mu\nu\rho\kappa}\rangle = E'\ \psi_{\mu\nu} .
\end{aligned} \tag{2-13}$$

Multiplying (2-8) on the left by $\varphi^{\mu*}$, and (2-13) on the left by $\varphi^{\mu*} \cdot \varphi^{\nu*}$, and integrating over the coordinates μ,ν, we find

$$E' = E \,. \tag{2-14}$$

Equations (2-8) and (2-13) are exactly the equations that Brenig obtained by multiplying the Schrödinger equation for $\Psi(1...A)$ by $\Pi^{\mu*}$ and $\Pi^{\mu\nu*}$ and integrating. Obviously, our variations of Π have the effect of excluding single-particle functions from this product. We could of course obtain the whole set of coupled integro-differential equations for the correlation functions by requiring that all the variations of $\langle \Pi | H | \Psi \rangle$ with respect to Π up to the Ath-order variation should vanish.

This is also evident from the fact that the energy E, evaluated in the form

$$E = \frac{\langle \Pi | H | \Psi \rangle}{\langle \Pi | \Psi \rangle} \,, \tag{2-15}$$

is independent of Π as long as Ψ is the true solution of the A-body Schrödinger equation.

In the independent-pair approximation the three- and four-particle correlations $\psi_{\mu\rho\kappa}$, $\psi_{\mu\nu\rho\kappa}$ in Eqs. (2-8) and (2-13) are replaced by suitably chosen products of one- and two-particle functions (see reference 1), and, after some straightforward algebra, the basic one- and two-particle equations of the independent-pair model are obtained. The one- and two-particle functions φ_μ and $\psi_{\mu\nu}$ that are obtained as solutions of these equations cannot be expected to make $\langle \Pi | H | \Psi \rangle$ exactly stationary to all orders of variations A. Nevertheless, the variations are due only to the independent-pair approximation. The better the independent-pair approximation, the more accurately should the first- and higher-order variations of $\langle \Pi | H | \Psi \rangle$ be equal

to zero. Since the independent-pair approximation is supposed to represent the two-particle correlations rather well,[8] the second variation should at least be small compared with higher ones. Considering $\langle \Pi | H | \Psi \rangle$ as a function of some single-particle parameter that determines the superscripted functions φ^{λ}, we can say that the solution of the one- and two-particle equations should be very near to a stationary value of $\langle \Pi | H | \Psi \rangle$ with as small a curvature as possible. This result has in fact been obtained by Mang and Wild in the three- and four-body case[4] and by the author in the five-body problem.[5] Hesse has compared the self-consistent solutions of Mang and Wild with the solutions he obtained by varying $\langle \Pi | H | \Psi \rangle$.[9] The minimum of $\langle \Pi | H | \Psi \rangle$ came to lie at a frequency of the single-particle oscillator ω that was very close to the self-consistent value of Mang and Wild. The value he obtained for the total energy E was of poorer accuracy, because the variational ansatz used was insufficiently flexible.

ACKNOWLEDGEMENTS

The author wishes to express his thanks to Professor F. Beck for having drawn his attention to the problem. The author is also grateful to the Lawrence Radiation Laboratory for a research contract, to the German Bundesministerium fur wissenschaftliche Forschung for a fellowship and to the Fulbright Commission for a travel grant.

APPENDIX

Remarks upon the Derivation of the One- and Two-Particle Equations

Introducing the independent-pair approximation in Eq. (2-8) we replace the three-particle function $\psi_{\mu\rho\kappa}$ by

$$\psi_{\mu\rho\kappa}(\mu\rho\kappa) = \varphi_\mu(\mu)\,\psi_{\rho\kappa}(\rho\kappa) - \varphi_\rho(\mu)\,\psi_{\mu\kappa}(\rho\kappa) - \varphi_\kappa(\mu)\,\psi_{\rho\mu}(\rho\kappa) \qquad \text{(A-1)}$$

retaining the correlation only between the coordinates ρ,κ that appear in the nucleon potential (see reference 1). In the integrals $\langle \varphi^\rho | T | \psi_{\mu\rho} \rangle$ the two-particle function $\psi_{\mu\rho}$ is replaced by the uncorrelated one, $\varphi_{\kappa\rho}$, since T is a one-particle operator (see reference 1). Thus, we obtain

$$\sum_\rho \langle \varphi^\rho | T | \psi_{\mu\rho} \rangle + \frac{1}{2} \sum_{\rho,\kappa} \langle \varphi^\rho \varphi^\kappa | v | \psi_{\mu\rho\kappa} \rangle - E\,\varphi_\mu \approx \sum_{\rho \neq \mu} \langle \varphi^\rho | T | \varphi_\rho \rangle \varphi_\mu(\mu)$$

$$- \sum_{\rho \neq \mu} \langle \varphi^\rho | T | \varphi_\mu \rangle \varphi_\rho(\mu) + \frac{1}{2} \sum_{\substack{\rho,\kappa \neq \mu \\ \rho \neq \kappa}} \{ \langle \varphi^\rho \varphi^\kappa | v | \psi_{\rho\kappa} \rangle \varphi_\mu(\mu) - \langle \varphi^\rho \varphi^\kappa | v | \psi_{\mu\kappa} \rangle \varphi_\rho(\mu)$$

$$- \langle \varphi^\rho \varphi^\kappa | v | \psi_{\rho\mu} \rangle \varphi_\kappa(\mu) \} - E\,\varphi_\mu \,. \qquad \text{(A-2)}$$

Introducing a single-particle energy ϵ_μ and a single-particle potential $V_{(\mu)}$

$$\epsilon_\mu = \langle \varphi^\mu | T | \varphi_\mu \rangle + \sum_\rho \langle \varphi^\mu \varphi^\rho | v | \psi_{\mu\rho} \rangle = E - \sum_{\rho \neq \mu} \langle \varphi^\rho | T | \varphi_\rho \rangle$$

$$- \frac{1}{2} \sum_{\rho,\kappa \neq \mu} \langle \varphi^\rho \varphi^\kappa | v | \psi_{\rho\kappa} \rangle \qquad \text{(A-3)}$$

$$V(\mu)\ \varphi_\mu(\mu) := \sum_\kappa \langle \varphi^\kappa(\kappa) | v(\mu\kappa) | \psi_{\mu\kappa}(\mu\kappa) \rangle ,$$

we can write (A-2) as

$$\sum_\rho \langle \varphi^\rho | T | \psi_{\mu\rho} \rangle + \frac{1}{2} \sum_{\rho,\kappa} \langle \varphi^\rho \varphi^\kappa | v | \psi_{\nu\rho\kappa} \rangle - E\ \varphi_\mu \approx -\epsilon_\mu \varphi_\mu - \sum_{\rho \neq \mu} \langle \varphi^\rho | T | \varphi_\mu \rangle \varphi_\rho(\mu)$$

$$- \sum_{\rho \neq \mu} \langle \varphi^\rho | V | \varphi_\mu \rangle \varphi_\rho(\mu) . \qquad \text{(A-5)}$$

Brening eliminates the distrubing nondiagonal matrix lements of (T + V) by assuming that a linear transformation of the superscripted functions φ^λ can be found so that all nondiagonal elements vanish. It is not completely trivial that such a transformation exists.

The variational method, however, shows a clear-cut way to circumvent the difficulty: Turning back to Eq. (2-7) we see that all the nondiagonal terms vanish automatically, if the variations $\delta\varphi^\mu$ are orthogonal to φ_ρ ($\rho = 1,\cdots,A;\ \rho \neq \mu$).

Since there are only a finite number of φ_ρ there must always be elements of the Hilbert space that are orthogonal to these φ_ρ. Assuming that we have chosen our variations $\delta\varphi^\mu$ in the subspace that is orthogonal to the φ_ρ's, we can trivially dispose of all the nondiagonal matrix elements.

REFERENCES

*Work done under the auspices of the U.S. Atomic Energy Commission.

1. W. Brenig, Nucl. Phys. 4, 363 (1957).
2. R. J. Eden, Proc. Roy. Soc. A235, 408 (1956)
3. R. J. Eden, V. J. Emergy, and S. Sampanthar, Proc. Roy. Soc. A253, 177 (1959), ibid. 186.
4. H. J. Mang and W. Wild, Z. Physik 154, 182 (1959).
5. K. Dietrich, Z. Physik 167, 563 (1962).
6. K. Dietrich, R. Folk, and H. J. Mang, Rutherford Jubilee International Conference 1961, to be published in Nucl. Phys. 49 (1963).
7. U. Gutsch, Nukleon-Wechselwirkung und leichte Hyperfragmente, Diplomarbeit, Universität Frankfurt/M, July 1963 (unpublished).
8. K. Kumar, Nucl. Phys. 21, 99 (1960).
9. K. Hesse, Behandlung des kernphysikalischen Drei-und Kerkörproblems in Paarnäherung mit Variations-ansatz. Diplomarbeit, Universität Frankfurt/M, March 1963 (unpublished)