SHORT-RANGE CORRELATIONS IN NUCLEAR WAVE FUNCTIONS

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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.

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It corresponds more closely to a large nucleus in the middle of the shell. Pairing of nucleons near the Fermi surface gives rise to long range correlations which can be ignored, however, in calculating bulk effects such as the binding energy per particle.

2. The Structure of the Wave Functions

It will be useful for the following to review at the outset certain well known features of the perturbation theory for non-degenerate bound states. The Rayleigh-Schrödinger perturbation series for the state Ψ and the energy shift ΔE can be obtained by iterating the following exact equations:

$$Z^{-\frac{1}{2}}\Psi = \Phi + (1 - \Lambda)(\mathscr{E}_0 - H_0)^{-1}(W - \Delta E)Z^{-\frac{1}{2}}\Psi, \tag{1}$$

$$\Delta E = (\Phi, WZ^{-\frac{1}{2}}\Psi), \tag{2}$$

$$Z = (\Phi, \Psi)^2, \tag{3}$$

where Φ is the zero order state satisfying the Schrödinger equation $(H_0 - \mathscr{E}_0)\Phi = 0$ and $(\Phi, \Phi) = 1$. The projection operator Λ projects into the state Φ . Eqs. (1) and (2) follow from the Schrödinger equation

$$(H+W)\Psi = (\mathscr{E}_0 + \Delta E)\Psi \tag{4}$$

and the coefficient Z is defined by eq. (3). Eqs. (1) and (2) yield a perturbation series for $Z^{-\frac{1}{2}}\Psi$ and for ΔE . The state vector Ψ itself can then be obtained from the condition $(\Psi, \Psi) = 1$.

We are interested in the case when H_0 is a shell model Hamiltonian and Φ is a shell model state, i.e. H_0 is additive in the nucleons and Φ is represented by a Slater determinant of single particle functions $\varphi_{\nu}(q)$. The letter q stands for the nucleon coordinates including charge- and spin coordinates. W is a two-body interaction. The state vector Ψ can then be expressed in the form

$$\Psi = Z^{\frac{1}{2}} \mathsf{F} \Phi, \tag{5}$$

where

$$\mathsf{F} = 1 + \sum_{k=1}^{A} \mathsf{F}_{k},\tag{6}$$

with

$$\mathsf{F}_{k} = (k!)^{-2} \int \mathrm{d}q_{1} \dots \int \mathrm{d}q_{k} \sum_{\nu_{1} \dots \nu_{k}} c^{\dagger}(q_{k}) \dots c^{\dagger}(q_{1})$$

$$(q_{1} \dots q_{k}|F_{k}|\nu_{k} \dots \nu_{1})c(\nu_{1}) \dots c(\nu_{k}). \tag{7}$$

The operators c(q) and $c^{\dagger}(q)$ respectively annihilate and create nucleons at the point q. They satisfy the usual commutation relations

$$\{c(q), c^{\dagger}(q')\} = \delta(q, q'). \tag{8}$$

The operator c(v) destroys a nucleon in the state v:

$$c(\nu) = \int dq \ c(q) \varphi_{\nu}^{*}(q). \tag{9}$$

The operator F_k by definition excites k nucleons from the zero order configuration into a superposition of excited configurations. The functions F_k therefore satisfy the orthogonality relation

$$\int dq_1 \varphi_{\nu}^*(q_1) (q_1 \dots q_k | F_k | \nu_k \dots \nu_1) = 0,$$
 (10)

where $\varphi_{\nu}(q)$ is any of the A single particle functions which occur in Φ .

One might expect that for a weak interaction W the state Φ approximates Ψ in the norm. In other words one might expect

$$||\Psi - \Phi||^2 = 2(1 - Z^{\frac{1}{2}}) \ll 1. \tag{11}$$

Actually this is not the case for large systems $^{2-4}$). For a Fermi gas of fixed density and a given interaction the constant Z tends to zero with increasing particle number A. This can easily be seen by examining the expression

$$Z^{-1} = 1 + \sum_{k} (k!)^{-2} \int dq_1 \dots \int dq_k \sum_{\nu_1 \dots \nu_k} |(q_1 \dots q_k)| F_k |\nu_k \dots \nu_1|^2.$$
 (12)

The functions F_k are antisymmetrized products of functions $(q_1 \dots q_l | S_l | \nu_l \dots \nu_1)$ such that the perturbation series for the S_l consists only of linked diagrams ¹²) †. These functions have the property

$$(l!)^{-2} \int dq_1 \dots \int dq_l \sum_{\nu_1 \dots \nu_l} |(q_1 \dots q_l | S_l | \nu_l \dots \nu_1)|^2 \lesssim \eta^{l-1} A, \qquad (13)$$

where η is some constant independent of A. In a Fermi gas with weak interaction we have $\eta \approx g^2(k_{\rm F}r_0)^3$ where g is a "coupling constant" measuring the strength of the interaction and the Fermi momentum $k_{\rm F}$ is the reciprocal range of the linked functions. Similarly all integrals over linked functions in eq. (12) are proportional to A. The relation between the F_k and the S_l is most easily stated in operator form l^2 :

$$F = e^{S}, (14)$$

with

$$S = \sum_{l=1}^{A} S_{l}. \tag{15}$$

The operator S_i is related to the function S_i by a relation of the form (7). The functions S_i satisfy the orthogonality relation (10). For the right hand side of

[†] This expansion of the functions F in antisymmetrized products is analogous to the Ursell expansion of the density matrix. See ref. 11).

eq. (12) one finds the following A-dependence of Z:

$$Z^{-1} = 1 + \sum_{p=2}^{A} \sum_{0 < n \le A/p} \frac{1}{n!} (C_p A)^n.$$
 (16)

Only integrals over $S_{p'}$ with $p' \leq p$ contribute to the coefficient C_p . For weak interactions we have $epC_p \ll 1$ and $\sum_p C_p$ converges to a constant C. Hence

$$Z \cong e^{-CA}. \tag{17}$$

In general we may say that the parameter η defined by eq. (13) measures the strength as well as the range of the correlations in the wave function.

The following discussions are based on the assumption $\eta \ll 1$. This assumption may be verified in perturbation theory for reasonably weak interactions. It can be expected, however, to hold also where a perturbation expansion of the S_t is not valid. For hard core potentials the S-functions must cancel the products of single particle functions at the core surface and drop off with increasing separation of the particles. In addition to the assumption $\eta \ll 1$ we shall assume that the largest eigenvalue of the matrix

$$(l!)^{-1} \int dq_1 \dots \int dq_l (q_1 \dots q_l | S_l | \nu_l \dots \nu_1) * (q_1 \dots q_l | S_l | \nu_l' \dots \nu'_1)$$
 (18)

is of order η^{l-1} or smaller. If these assumptions are valid one can always make the integral

$$\int \! \mathrm{d}q \sum_{\nu} |(q|S_1|\nu)|^2$$

as small as desired by an appropriate choice of the single particle functions. Consider for instance

$$\Psi = Z_0^{\frac{1}{2}} e^{S^{(0)}} \Phi^{(0)}, \tag{19}$$

with $S_1^{(0)} \neq 0$ and define the Slater determinant $\Phi^{(1)}$ by

$$e^{\mathbf{S}_{\mathbf{1}}^{(0)}} \mathbf{\Phi}^{(0)} = \text{const. } \mathbf{\Phi}^{(1)}, \quad (\mathbf{\Phi}^{(1)}, \mathbf{\Phi}^{(1)}) = 1.$$
 (20)

Like any other state, the state $e^{S^{(0)}-S_1^{(0)}}\Phi^{(1)}$ may be represented in the form

$$e^{S^{(0)}-S_1^{(0)}}\Phi^{(1)} = \text{const. } e^{S^{(1)}}\Phi^{(1)}.$$
 (21)

From this equation one can calculate $S_k^{(1)}$ in terms of the functions $S_p^{(0)}$ by expansion in powers of η . In zeroth order we have

$$(q_1|S_1^{(1)}|q_2) = \int dq'_1 \int dq'_2 \int dq_3 \int dq'_3 (q_1|1 - A^{(1)}|q'_1)$$

$$\times (q'_3|A^{(1)}|q_3) (q'_2|A^{(1)}|q_2) (q'_1 q_3|S_2^{(0)}|q'_3 q'_2)$$
(22)

and

$$(q_1q_2|S_2^{(1)}|q_3q_4) = \int dq'_1 \dots \int dq'_4(q_1|1 - \Lambda^{(1)}|q'_1) \times (q_2|1 - \Lambda^{(1)}|q'_2)(q'_1q'_2|S_2^{(0)}|q'_3q'_4)(q'_3|\Lambda^{(1)}|q_3)(q'_4|\Lambda^{(1)}|q_4), \quad (23)$$

where

$$(q_1q_2|S_2|q_3q_4) \equiv \sum_{\nu_1\nu_2} (q_1q_2|S_2|\nu_2\nu_1) \varphi_{\nu_2}^*(q_3) \varphi_{\nu_1}^*(q_4), \tag{24}$$

and

$$(q'|A^{(1)}|q) \equiv \sum_{\nu} \varphi_{\nu}^{(1)}(q')\varphi_{\nu}^{(1)*}(q).$$
 (25)

If $S_1^{(1)}$ is not small enough the procedure can be repeated defining $\Phi^{(2)}$ by

$$e^{\mathbf{S}_{1}^{(1)}} \mathbf{\Phi}^{(1)} = \text{const. } \mathbf{\Phi}^{(2)}.$$
 (26)

In the following we shall therefore assume $S_1 = 0$. This assumption governs the choice of the single particle wave functions. It is a generalization of the Hartree-Fock condition.

In general our wave function $Z^{-\frac{1}{2}}\Psi$ is well approximated by the Slater determinant Φ if all nucleons are farther apart than a "healing distance" ⁵) h which may be defined by

$$h \equiv \left(\eta \rho^{-1} \frac{3}{4\pi}\right)^{\frac{1}{3}},\tag{27}$$

where ρ is the nucleon density. For smaller distances the corrections described by the cluster functions S_k may be large. Wave functions with such a structure have been widely used ^{13–18}). The "superposition wave function" of the form

$$\Psi_{r}(q_{1} \dots q_{A}) = \mathscr{A}_{\nu} \left[\left(1 + f_{\nu_{1} \nu_{3}}(q_{1} q_{2}) \right) \left(1 + f_{\nu_{1} \nu_{3}}(q_{1} q_{3}) \right) \dots \right. \\ \left. \times \left(1 + f_{\nu_{4} \nu_{3}}(q_{2} q_{3}) \right) \dots \left(1 + f_{\nu_{A-1} \nu_{A}}(q_{A-1}, q_{A}) \right) \varphi_{\nu_{1}}(q_{1}) \dots \varphi_{\nu_{A}}(q_{A}) \right]$$
(28)

has these properties if the quantities f vanish outside the healing distance. The symbol \mathscr{A}_{ν} indicates antisymmetrization with respect to ν . It is therefore of interest to establish the relation between the functions f and our cluster functions S_k . These relations follow in a straightforward manner from eq. (28) and

$$\Psi_f = (\Phi, \Psi_f) e^{S_f} \Phi. \tag{29}$$

Simple explicit expressions are obtained by expansion in powers of η . The zero order term in S_{Π} vanishes. In first order we have

$$(q|S_{I1}^{(1)}|\nu) = \sum_{\nu'} \int dq' \int dq'' (q|1-\Lambda|q') \varphi_{\nu}^{*}(q'') \mathscr{A}_{\nu} f_{\nu\nu'}(q', q'') \varphi_{\nu}(q') \varphi_{\nu'}(q'')$$
(30)

where Λ is the projection into the occupied single particle states:

$$(q|\Lambda|q') = \sum_{\nu} \varphi_{\nu}(q)\varphi_{\nu}^{*}(q'). \tag{31}$$

Most authors $^{17-13}$) assume only one function f independent of the single particle states. De Shalit and Weisskopf 18) have state-dependent functions f

which satisfy the orthogonality relation

$$\int dq' \varphi_{\nu}^*(q') f_{\nu_1 \nu_2}(q', q) \varphi_{\nu_1}(q') \varphi_{\nu_2}(q) = 0.$$
 (32)

In that case $S_{f1}^{(1)}$ vanishes and the first non-vanishing contribution to S_{f1} is of order η^2 . The zero order term in S_{f2} is, as one should expect,

$$\begin{split} &(q_1q_2|S_{f_2}^{(0)}|\nu_2\nu_1)\\ &= \int \mathrm{d}q'_1 \int \mathrm{d}q'_2(q_1|1-\varLambda|q'_1)(q_2|1-\varLambda|q'_2) \mathscr{A}_\nu f_{\nu_1\nu_2}(q'_1q'_2)\varphi_{\nu_1}(q'_1)\varphi_{\nu_2}(q'_2) \end{split} \tag{33}$$

and to first order in η one finds

$$\begin{split} (q_1q_2|S_{f_2}^{(1)}|\nu_2\nu_1) &= \int \mathrm{d}q'_3 \sum_{\nu_3} \varphi_{\nu_3}^*(q'_3) \int \mathrm{d}q'_1 \int \mathrm{d}q'_2 (q_1|1-A|q'_1) (q_2|1-A|q'_2) \\ &\times \mathscr{A}_{\nu} \{ f_{\nu_1\nu_3}(q'_1q'_3) f_{\nu_1\nu_3}(q'_1q'_2) f_{\nu_2\nu_3}(q'_2q'_3) + f_{\nu_1\nu_3}(q'_1q'_3) f_{\nu_2\nu_3}(q'_2q'_3) \\ &+ f_{\nu_1\nu_2}(q'_1q'_2) f_{\nu_1\nu_3}(q'_1q'_3) + f_{\nu_2\nu_3}(q'_2q'_3) f_{\nu_1\nu_3}(q'_1q'_2) \} \\ &\times \varphi_{\nu_1}(q'_1) \varphi_{\nu_2}(q'_2) \varphi_{\nu_3}(q'_3). \end{split} \tag{34}$$

The last two terms between braces vanish if the orthogonality condition (32) is satisfied.

3. The Schrödinger Equation

In our representation the Schrödinger equation takes the form

$$He^{S}\Phi = Ee^{S}\Phi. \tag{35}$$

There follows an expression for the binding energy E:

$$E = (\Phi, e^{-S}He^{S}\Phi) = (\Phi, (H+[H, S_2])\Phi). \tag{36}$$

In the last step it is assumed that $S_1 = 0$ and H contains only two body forces. There follows further from eq. (35) a set of coupled equations for the cluster functions:

$$(c(v_1) \dots c(v_k)\mathbf{\Phi}, a(q_1) \dots a(q_k)e^{-\mathbf{S}}He^{\mathbf{S}}\mathbf{\Phi}) = 0, \tag{37}$$

where

$$a(q) = \int\!\!\mathrm{d}q'(q|\mathbf{I}-A|q')c(q').$$

The perturbation solution of these equations for $H=H_0+W$ and $H_0\Phi=\mathscr{E}_0\Phi$ has been discussed elsewhere ¹²). Even if this straightforward perturbation theory is not applicable expansion in powers of η provides a basis for a systematic approximation. In the lowest approximation the equations k=2 and k=1 are independent of S_3 and higher cluster functions. A hard core repulsion presents no serious difficulty provided the core radius is small compared to the average distance between particles. The equations k=2 and k=1 may be used with

the condition $S_1 = 0$ to determine the single particle functions φ_{ν} and the two-body cluster functions S_2 . The equation is essentially the Bethe-Goldstone equation ¹⁹). The Bethe-Goldstone wave functions are in our notation

$$(q_1 q_2 | \psi | \nu_2 \nu_1) = \mathscr{A}_{\nu} \varphi_{\nu_1}(q_1) \varphi_{\nu_2}(q_2) + (q_1 q_2 | S_2 | \nu_2 \nu_1). \tag{38}$$

The equations (35) are equivalent to the system of equations for the functions

$$(q_1 \ldots q_k | \psi_k | \nu_k \ldots \nu_1) = (c(\nu_k) \ldots c(\nu_1) \mathbf{\Phi}, c(q_1) \ldots c(q_k) Z^{-\frac{1}{2}} \mathbf{\Psi}), \tag{39}$$

which have been discussed by Brenig ²⁰). The problem of finding approximate solutions for eqs. (37) will be treated in detail in a subsequent article.

4. The Density Matrices

While the energy formula (36) involves only S_2 , the knowledge of higher cluster functions is necessary according to eq. (16) to obtain the normalized wave function. One might therefore suspect that our approximations are capable of giving approximate expressions for the energy only and not for the expectation values of other operators. Nevertheless we propose to show that approximate expressions for the density matrices can be obtained by expansion in powers of η .

The one-particle density matrix is defined by

$$(q|\rho|q') = \int dq_2 \dots \int dq_A \Psi(q_1 q_2 \dots q_A) \Psi^*(q'_1 q_2 \dots q_A)$$

$$= A^{-1}(\mathbf{\Phi}, e^{\mathbf{S}\dagger} e^{\mathbf{S}} \mathbf{\Phi})^{-1}(\mathbf{\Phi}, e^{\mathbf{S}\dagger} c^{\dagger}(q') c(q) e^{\mathbf{S}} \mathbf{\Phi}).$$

$$(40)$$

In the evaluation of the ratio (40) the denominator will cancel out and a good approximation can be obtained which involves S_2 only.

It is convenient to define operators b by

$$b^{\dagger}(q) = \int dq'(q|\Lambda|q')c(q'),$$

$$b^{\dagger}(\nu) = c(\nu).$$
(41)

where Λ is the projection operator (31). The operator $b^{\dagger}(v)$ creates a "hole" in the state v. To evaluate expression (40) we replace c(q) everywhere by $a(q) + b^{\dagger}(q)$ and shift all annihilation operators to the right and creation operators to the left. The relevant relations are

$$c^{\dagger}(q')c(q) = (q|\Lambda|q') + a^{\dagger}(q')b^{\dagger}(q) + b(q')a(q) + a^{\dagger}(q')a(q) - b^{\dagger}(q)b(q') \quad (42)$$

and

$$a(q)e^{S}\Phi = [a(q), S]e^{S}\Phi, \quad b(q)e^{S}\Phi = [b(q), S]e^{S}\Phi.$$
 (43)

There follows

$$(q|\rho|q') = A^{-1}(q|A|q')$$

$$+A^{-1}(\Phi, e^{S\dagger}e^{S}\Phi)^{-1}(\Phi, e^{S\dagger}([a(q'), S]^{\dagger}\{[b(q), S]^{\dagger}+[a(q), S]\}$$

$$-\{[a(q), S]+[b(q), S]^{\dagger}\}[b(q'), S]$$

$$+\{b(q'), [a(q)S]\}+\{[a(q'), S], b(q)\}^{\dagger})e^{S}\Phi).$$

$$(44)$$

Re-ordering and successive application of eqs. (43) produces multiple integrals over linked products of the cluster functions S_k . The largest correlation correction to the density matrix $(q|\rho|q')$ come from terms which are bilinear in S_2 . Let $(q|g_1|q')$ be defined by

$$(q|\rho|q') = A^{-1}((q|\Lambda|q') + (q|g_1|q')). \tag{45}$$

We find in first approximation for g_1

$$\begin{split} (q|g_1|q') &= \frac{1}{2} \int \mathrm{d}q'' \sum_{\nu_1 \nu_2} (qq''|S_2|\nu_2 \nu_1) (q'q''|S_2|\nu_2 \nu_1)^* \\ &- \frac{1}{2} \int \mathrm{d}q_1 \int \mathrm{d}q_2 \sum_{\nu} (q_1 q_2|S_2|\nu q') (q_1 q_2|S_2|\nu q)^*, \end{split} \tag{46}$$

where

$$(q_1 q_2 | S_2 | \nu q) \equiv \sum_{\nu'} (q_1 q_2 | S_2 | \nu \nu') \varphi_{\nu'}^*(q). \tag{47}$$

We see that the order of magnitude of the correction to the one-particle density matrix may be measured by the integral

$$\int dq \int dq' |\langle q|g_1|q'\rangle|^2 \approx \eta^2 A. \tag{48}$$

Neglected terms contribute only higher powers of η . For the zero order term the corresponding expression is

$$\int dq \int dq' |\langle q|\Lambda|q \rangle|^2 = \int dq \langle q|\Lambda|q \rangle = A.$$
(49)

The same techniques may be used to calculate the two-particle density matrix:

$$(q_{1}q_{2}|\rho|q'_{2}q'_{1}) = \int dq_{3} \dots \int dq_{A} \Psi(q_{1}q_{2} \dots q_{A}) \Psi^{*}(q'_{1}q'_{2}q_{3} \dots q_{A})$$

$$= \frac{1}{A(A-1)} (\mathbf{\Phi}, e^{\mathsf{S}\dagger}e^{\mathsf{S}}\mathbf{\Phi})^{-1}(\mathbf{\Phi}, e^{\mathsf{S}\dagger}c^{\dagger}(q'_{2})c^{\dagger}(q'_{1})c(q_{1})c(q_{2})e^{\mathsf{S}}\mathbf{\Phi}).$$
(50)

Upon re-ordering the creation and annihilation operators we have

$$\begin{aligned} (q_1 q_2 | \rho | q'_2 q'_1) &= \frac{1}{A (A - 1)} \{ \mathscr{A}(q_1 | A | q'_1) (q_2 | A | q'_2) \\ &+ \mathscr{A}(q_1 | A | q'_1) (q_2 | g_1 | q'_2) + (q_1 q_2 | g_2 | q'_2 q'_1) \}. \end{aligned}$$
 (51)

The definition of g_2 is implied in this equation, neglecting all contributions involving higher cluster functions and higher powers of S_2 we find for g_2 :

$$(q_{1}q_{2}|g_{2}|q'_{2}q'_{1}) = (q_{1}q_{2}|S_{2}|q'_{2}q'_{1}) + (q'_{1}q'_{2}|S_{2}|q_{2}q_{1})^{*}$$

$$+ \frac{1}{2} \int dq' \int dq'' (q'q''|S_{2}|q'_{2}q'_{1}) (q'q''|S_{2}|q_{2}q_{1})^{*}$$

$$+ \frac{1}{2} \sum_{\nu'\nu'} (q_{1}q_{2}|S_{2}|\nu''\nu') (q'_{1}q'_{2}|S_{2}|\nu''\nu')^{*}$$

$$- \mathcal{A} \int dq \sum_{\nu} (qq_{1}|S_{2}|q'_{2}\nu) (qq'_{1}|S_{2}|q_{2}\nu)^{*},$$

$$(52)$$

where

$$(q_1q_2|S_2|q'_2q'_1) \equiv \sum_{\nu_2,\nu_1} (q_1q_2|S_2|\nu_2\nu_1)\varphi_{\nu_2}^*(q'_2)\varphi_{\nu_1}^*(q_1). \tag{53}$$

The first two terms in eq. (50) give a contribution of order η A to

$$\frac{1}{4} \int dq_1 \int dq_2 \int dq'_1 \int dq'_2 |(q_1 q_2 | g_2 | q'_2 q'_1)|^2.$$
 (54)

The remaining terms give contributions of order $\eta^2 A$. The approximate density matrices (45) and (51) yield respectively approximations for the expectation values of one- and two-particle operators. Whether or not higher order correction terms are indeed negligible depends on the operators involved and must be examined in each case.

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