

Spin-Orbit Coupling and Tensor Forces

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The possible explanation of the spin-orbit coupling, in heavy nuclei, by second-order effects of the tensor forces is investigated. The various second order terms are described by 4 graphs, in the case of one particle outside closed shells. The main contribution comes from an exclusion effect: two particles of the closed shells cannot, by mutual excitation, jump into the orbit which is already occupied by the outside particle. This effect could account, at least partially, for the observed spin-orbit splitting. The case of a hole is also investigated, and shows the same kind of agreement. A comparison with other works is discussed.

§ 1. Introduction

It is very likely that the properties of complex nuclei could in principle be computed from the two-body forces between nucleons. The spin-orbit coupling in complex nuclei, which is so important in the shell model, should be explained in terms of non-central two-body forces.

The existence of mutual spin-orbit forces in the two-body interaction is still under discussion. Such forces, in addition to the usual central and tensor ones, are sufficient to explain the two-body scattering and polarization data,^{1,2)} but there was raised some doubt whether these spin-orbit forces are actually necessary, and it was recently claimed that central and tensor forces, with hard cores, could suffice.³⁾

A related problem arises in the consideration of complex nuclei. Two-body spin-orbit forces could account for the shell-model spin-orbit splitting; a first-order perturbation calculation is perhaps too crude, but a more refined calculation,⁴⁾ using the reaction matrix, could pretend to quantitative results. On the other hand, it was attempted to use only tensor forces; since tensor forces give no splitting in first-order perturbation theory, second-order effects had to be computed. For light nuclei, it was found that tensor forces could account for an important fraction of the observed splittings.^{5,6)} But, in the case of heavy nuclei, a calculation in a previous paper,⁷⁾ using the reaction matrix as an intermediate step, predicted a much too small effect of the tensor forces.

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The purpose of the present paper is to emphasize the general importance of some exclusion effects which might escape a calculation based on the use of an approximate reaction matrix, and to apply these considerations to the effects of tensor forces in the spin-orbit splitting of heavy nuclei.* It will be found that these exclusion effects might indeed be important and account, at least partially, for the observed splittings. The general formulation of the problem, for one particle outside the closed shells, is reviewed in § 2. § 3 describes an approximate procedure to reduce the problem to a calculation of the Thomas-Fermi kind. This calculation is actually carried out in § 4 and the results are compared with the experimental data. The case of one hole in the closed shells is studied in § 5. The conclusions are stressed in § 6.

§ 2. Energies of nuclei

The general prescription for computing the first levels of a nucleus made of closed shells plus some particles or holes has been given by Bloch and Horowitz.⁸⁾ We here consider the special case of one particle outside the closed shells (the case of one hole will be very similarly treated in § 5). The total hamiltonian is

$$H = H_0 + V, \quad (1)$$

where H_0 is some zeroth-order hamiltonian and V is the residual interaction. V causes a total energy shift of the nucleus

$$\Delta E = \Delta E^c + \Delta E^p. \quad (2)$$

ΔE^c is the contribution of the closed shells and does not depend on the presence of outside particles. ΔE^p is the contribution of outside particles. This separation is actually just a matter of convenient definition, and some terms of ΔE^p may alternatively be thought of as involving particles in the closed shells. ΔE^p is implicitly given by a Brillouin-Wigner perturbation series as follows: A vacuum state $|0\rangle$ is defined as the unperturbed closed shell nucleus. Other eigenstates of H_0 are conveniently described by using annihilation and creation operators η and η^\dagger ; the unperturbed nucleus with one particle outside the closed shells is therefore in the state $\eta^\dagger|0\rangle$ with an energy E_0 . ΔE^p is then conveniently described as a sum of graphs⁹⁾

$$\Delta E^p = \langle 0 | \eta_p \Phi \eta_p^\dagger | 0 \rangle = \left\langle 0 \left| \eta_p V \sum_{n=0}^{\infty} \left(\frac{Q_0}{E_0 + \Delta E^p - H_0} V \right)^n \eta_p^\dagger | 0 \right\rangle_L, \quad (3)$$

where L means that only linked graphs are included and where Q_0 is the projector

* In the case of light nuclei, these exclusion effects, although they had already been implicitly taken into account in Ref. 5), were explicitly shown to be important, in Ref. 6) for the bound state problem, and in Ref. 6 bis) for the He⁴-neutron scattering problem. The spin-orbit coupling at low energy could then be explained by strong tensor forces.

outside the subspace of the unperturbed states with an energy E_0 , i. e., the intermediate states represented by one particle line.*

(3) is exact. A second-order approximation, in which ΔE^P is neglected in the energy denominator, is

$$\Delta E^P = \langle 0 | \eta_P \left[V + V \frac{Q_0}{E_0 - H_0} V \right] \eta_P^\dagger | 0 \rangle. \quad (4)$$

This expression is nothing but the usual second order perturbation result. The main advantage of having used the language of graphs is to clearly exhibit all possible exchange effects. If V consists of two-body interactions, represented by a horizontal dotted line, the second-order terms in (4) are represented by the four graphs of Fig. 1, which we shall now discuss in some detail.

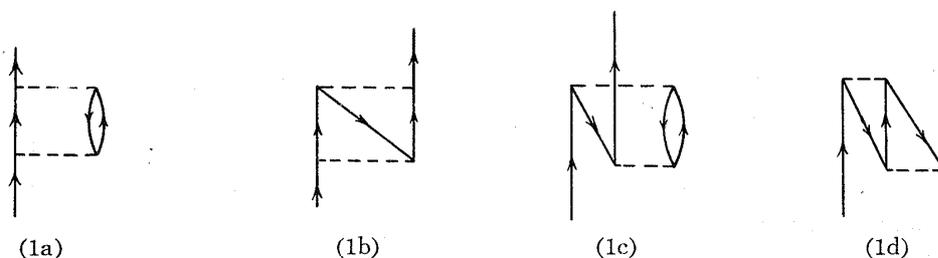


Fig. 1. The second-order graphs for one particle.

Graphs (1a) and (1b) are the direct and exchange second-order terms of the reaction matrix for interactions between the outside particle and one of the particles in the closed shells. These graphs appear in a naive extension of the Brueckner method to the degenerate nuclei. They were considered by many authors for various kinds of problems. If we are interested in the spin-orbit splitting which appears from (4) when V contains tensor forces, graphs (1a) and (1b) correspond to these terms which were considered in I, where it was shown that their contribution to the spin-orbit splitting is small.

Graphs (1c) and (1d) describe exclusion effects involving two core particles. By mutual interaction, two particles in the closed shells can get excited to intermediate states; but the state $\eta_P^\dagger | 0 \rangle$ already occupied by the outside particle is not available. This effect can be visualized before the elimination of disconnected graphs by saying that the graphs of Fig. 2 are forbidden by the Pauli principle. It is easy to see that graphs (1c) and (1d) provide the necessary subtraction. This modification of the reaction matrix for a pair of particles in the closed shells, because of the presence of an outside particle, would escape calculations based on an approximate reaction matrix computed beforehand for two particles imbedded in infinite nuclear matter, an approximate procedure which was often used.¹⁰⁾ Because

* The states $\eta_P^\dagger | 0 \rangle$ which differ by spin or orbital angular momentum orientation are degenerate, and this proper linear combination must be chosen which diagonalizes \mathcal{O} .



Fig. 2. The excluded graphs.

of such approximations, graphs (1c) and (1b) did not appear in I. The main purpose of the present paper is to investigate these graphs and to show their importance.

We shall therefore proceed to compute the contribution to (4) of graph (1c), which is

$$\langle P | \mathcal{U}^{(c)} | P \rangle \equiv \Delta E^{P(c)} = \sum_{m,n,s} \frac{\langle mn | v | Ps \rangle \langle Ps | v | mn \rangle}{E_p + E_s - E_m - E_n}, \quad (5)$$

where P, m, n, s are single particle states; E_p, E_s, E_m, E_n are the corresponding single particle energies; and v is the two-body interaction. The summation is on unoccupied states s and on occupied closed shell states m and n .

§ 3. Reduction of the problem to a Fermi-gas calculation

If the interactions v are central and tensor forces, only the term of (4) which contains twice the tensor force will contribute to the spin-orbit splitting. The tensor force between nucleons i and j is

$$v = A[1 - \chi + \chi(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)]u(r)S_{ij}(\mathbf{r}), \quad (6)$$

where

$$S_{ij}(\mathbf{r}) = 3(\boldsymbol{\sigma}_i \cdot \mathbf{r})(\boldsymbol{\sigma}_j \cdot \mathbf{r})/r^2 - (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j). \quad (7)$$

We shall now make some approximation of the same kind as in I.* If we took all intermediate states as plane waves, the spin-orbit potential would vanish, because there is no spin-orbit potential in a constant density medium. Since, however, we are considering large nuclei, we shall assume the minimum departure from plane waves, which gives a non-vanishing result: intermediate particle states such as $|s\rangle$ will be chosen as plane waves; and similarly for the hole states $|m\rangle$ (the normalization of these plane waves will be chosen to be unity in the unit volume). In order to obtain a finite result, we must take one of the hole states different from a plane wave, and it can be seen that this hole state must be $|n\rangle$. The momentum representatives $\langle \mathbf{k}_n | n \rangle$

* The numerical factors in the definitions of the present paper and the notations may differ from those used in I.

and $\langle \mathbf{k} | P \rangle$ will, however, be strongly peaked, so that E_n and E_P may be replaced by $k_n^2/2M$ and $k^2/2M$. With all these simplifications, (5) may be rewritten in a momentum representation

$$\langle \mathbf{k}' | \psi^{(c)} | \mathbf{k} \rangle = \sum_{\substack{n \\ \text{occupied}}} \frac{2M}{(2\pi)^{12}} \int d^3 \mathbf{k}_n' \int d^3 \mathbf{k}_n \int_{k_m < k_0} d^3 \mathbf{k}_m \int_{k_s > k_0} d^3 \mathbf{k}_s$$

$$\langle n | \mathbf{k}_n \rangle \langle \mathbf{k}_n' | n \rangle \frac{\langle \mathbf{k}_m \mathbf{k}_n | v | \mathbf{k} \mathbf{k}_s \rangle \langle \mathbf{k}' \mathbf{k}_s | v | \mathbf{k}_m \mathbf{k}_n' \rangle}{k^2 + k_s^2 - k_m^2 - k_n^2}. \quad (8)$$

In other words, at each point the closed shell core is pictured as a local Fermi gas. The summations on occupied or unoccupied states are performed on momenta smaller or greater than the local Fermi momentum k_0 , which is a function of the position \mathbf{r} :

$$\rho(r) = (2/3\pi^2) k_0^3. \quad (9)$$

The mixed density function is approximated by one of this local Fermi gas:

$$\sum_{\substack{n \\ \text{occupied}}} \langle \mathbf{r} | n \rangle \langle n | \mathbf{r}' \rangle = \rho(r) (3/4\pi k_0^3) \int_{\kappa < k_0} d^3 \boldsymbol{\kappa} \exp[-i \boldsymbol{\kappa} \cdot (\mathbf{r}' - \mathbf{r})]; \quad (10)$$

transforming (10) to the momentum representation we obtain

$$\sum_{\substack{n \\ \text{occupied}}} \langle \mathbf{k}_n' | n \rangle \langle n | \mathbf{k}_n \rangle = (2\pi)^3 \int d^3 \mathbf{r} \exp[i(\mathbf{k}_n - \mathbf{k}_n') \cdot \mathbf{r}] \rho(r) (3/4\pi k_0^3) \varepsilon(k_0 - k_n), \quad (11)$$

where ε is the step function.

We shall only keep in the v matrix element product of (8) that term which is linear in the spin $\boldsymbol{\sigma}$ of the \mathbf{k} or \mathbf{k}' states, and scalar in the isotopic spin, since that term is the only one which contributes to the spin-orbit splitting:

$$\langle \mathbf{k}_m \mathbf{k}_n | v | \mathbf{k} \mathbf{k}_s \rangle \langle \mathbf{k}' \mathbf{k}_s | v | \mathbf{k}_m \mathbf{k}_n' \rangle = 9iA^2 (2\pi)^6 (1 - 2\chi + 4\chi^2) \delta(\mathbf{k}_m + \mathbf{k}_n - \mathbf{k} - \mathbf{k}_s)$$

$$\delta(\mathbf{k}' + \mathbf{k}_s - \mathbf{k}_m - \mathbf{k}_n') \boldsymbol{\sigma} \cdot [(\mathbf{k}_n' - \mathbf{k}_s) \times (\mathbf{k}_n - \mathbf{k}_s)] \frac{(\mathbf{k}_n' - \mathbf{k}_s) \cdot (\mathbf{k}_n - \mathbf{k}_s)}{|\mathbf{k}_n' - \mathbf{k}_s|^2 |\mathbf{k}_n - \mathbf{k}_s|^2}$$

$$\times w(|\mathbf{k}_n' - \mathbf{k}_s|) w(|\mathbf{k}_n - \mathbf{k}_s|) + \dots, \quad (12)$$

where

$$w(k) = 4\pi \int_0^\infty j_2(kr) u(r) r^2 dr \quad (13)$$

(j_2 is the spherical Bessel function¹¹).

In a large nucleus, the outside particle undergoes only small angle scatterings when propagating through nuclear matter. Therefore $\mathbf{k}' - \mathbf{k}$ and, because of the δ functions in (12),

$$\mathbf{g} = \mathbf{k}_n' - \mathbf{k}_n \quad (14)$$

are small quantities; we shall expand (12) into a series of \mathbf{g} , keeping only the first non-vanishing term which is

$$\langle \mathbf{k}_m \mathbf{k}_n | v | \mathbf{k} \mathbf{k}_s \rangle \langle \mathbf{k}' \mathbf{k}_s | v | \mathbf{k}_m \mathbf{k}_n \rangle = 9iA^2 (2\pi)^6 (1 - 2\chi + 4\chi^2) \delta(\mathbf{k}' - \mathbf{k} - \mathbf{g}) \\ \delta(\mathbf{k}_m + \mathbf{k}_n - \mathbf{k} - \mathbf{k}_s) \boldsymbol{\sigma} \cdot [\mathbf{g} \times (\mathbf{k} - \mathbf{k}_m)] \frac{[\tau\omega(|\mathbf{k} - \mathbf{k}_m|)]^2}{|\mathbf{k} - \mathbf{k}_m|^2}. \quad (15)$$

Using now (11), (14) and (15) in (8), we obtain

$$\langle \mathbf{k}' | \mathcal{V}^{(e)} | \mathbf{k} \rangle = \int d^3 \mathbf{r} e^{i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}} \boldsymbol{\sigma} \cdot (\mathbf{r} \times \mathbf{k}) \frac{1}{r} \frac{d}{dr} a^{(e)} \rho \quad (16)$$

where

$$a^{(e)} = (1 - 2\chi + 4\chi^2) \frac{27MA^2}{16\pi^4 k_0^3 k^2} \int_{k_n < k_0} d^3 \mathbf{k}_n \int_{k_m < k_0} d^3 \mathbf{k}_m \int_{k_s > k_0} d^3 \mathbf{k}_s \delta(\mathbf{k} + \mathbf{k}_s - \mathbf{k}_m - \mathbf{k}_n) \\ \frac{\mathbf{k} \cdot (\mathbf{k}_m - \mathbf{k})}{k^2 + k_s^2 - k_m^2 - k_n^2} \frac{[\tau\omega(|\mathbf{k}_m - \mathbf{k}|)]^2}{|\mathbf{k}_m - \mathbf{k}|^2}. \quad (17)$$

From (16) and (17) it is seen that graph (1c) contributes an effective spin-orbit coupling with a radial dependence $(1/r)(d/dr)a^{(e)}\rho$. Strictly speaking, $a^{(e)}$ is a function of k and of r (through k_0). However, in the case where $a^{(e)}$ does not depend too strongly on r , (16) is the familiar $a^{(e)}(1/r)(d\rho/dr)(\boldsymbol{\sigma} \cdot \mathbf{l})$ spin-orbit coupling. Here we are interested in the spin-orbit potential acting on a bound particle with an energy just above the last closed shell; the momentum k of this particle will be replaced by the Fermi momentum k_0 as an average value.

In the case where the even and odd tensor forces are given by different w functions, the even and odd contributions add together without interference.

§ 4. Practical calculation of the spin-orbit potential magnitude and comparison with experiment

The magnitude of the term (1c) of the spin-orbit potential can be computed without further approximations, by the same techniques as in I. We choose as integration variables $\mathbf{K} = \mathbf{k}_m - \mathbf{k}$, \mathbf{k}_s , \mathbf{k}_n , and obtain

$$a^{(e)} = (1 - 2\chi + 4\chi^2) \frac{27MA^2}{32\pi^4 k_0^3} \int_{|\mathbf{K} - \mathbf{k}| > k_0} d^3 \mathbf{K} \frac{\mathbf{k} \cdot \mathbf{K}}{k^2} \frac{\omega^2(K)}{K^2} \int_{\substack{|\mathbf{k}_s + \mathbf{K}| > k_0 \\ k_s < k_0}} d^3 \mathbf{k}_s \frac{1}{(\mathbf{k} - \mathbf{k}_s) \cdot \mathbf{K} - K^2}. \quad (18)$$

We successively perform the integrals on \mathbf{k}_s and on the angles of \mathbf{K} ; it is necessary to subdivide \mathbf{k} and \mathbf{K} spaces into regions. The result of these integrations is a "universal" function $2\pi^2 k_0 C(K, k)$ which is given in the Appendix for the case $k = k_0$, appropriate to the last bound nucleon. The last integration on K must be done numerically:

$$a^{(c)} = (1 - 2\chi + 4\chi^2) \frac{27MA^2}{16\pi^2 k_0^2 k} \int_{k-k_0}^{k+k_0} dK \cdot KC(K, k) w^2(K). \quad (19)$$

(19) was actually computed (with $k=k_0$) for the Gammel-Thaler¹⁾ and the second-order meson theory³⁾ tensor potentials, the Bessel transforms (13) of which can be calculated analytically. No hard core was taken into account; it may be noted, however, that any Fourier component with a momentum higher than $2k_0$ would not affect (19). k_0 is related by (9) to the local density and should vary throughout the nuclear surface; $a^{(c)}$ was actually computed for several values of k_0 , but appears to be not very sensitive to k_0 (the value of k_0 which corresponds to the average density of nuclear matter is about $1.27 \times 10^{13} \text{ cm}^{-3}$). The results are tabulated in Table I. We see that $a^{(c)}$ depends somewhat on the tensor force, but is always of the same order of magnitude.

The experimental strength of the spin-orbit coupling in heavy nuclei is a bit confusing. The doublet splittings in Pb^{207} and Pb^{209} can be explained¹²⁾ by a spin orbit force $a(1/r)(d\rho/dr)(\sigma \cdot l)$ with $a \sim 57 \text{ Mev } (10^{-13} \text{ cm})^5$. But values of a four times greater were suggested to be necessary to account for the sequence of the single-particle levels in an average potential¹³⁾. The former evidence, from doublet splittings, is perhaps to be preferred, since it is more direct. It must also be remembered that the relation between a and the doublet splitting is extremely sensitive to detailed assumptions about the nuclear surface and the radial wave functions. For all these reasons, we cannot hope to check the agreement beyond mere orders of magnitude.

In a second-order calculation, the value of a would be the sum of the contributions from the four graphs of Fig. 1. It was shown in I that graphs (1a) and (1b) give a negligible contribution.* From Table I, it appears that the contribution

Table I. The value of the spin-orbit constant contribution $a^{(c)}$.

Tensor force	k_0 10^{13} cm^{-3}	$a^{(c)}$ Mev $(10^{-13} \text{ cm})^5$
Gammel-Thaler	1.27	30
	1.05	37
	0.87	41
2nd-order meson theory	1.27	50
	0.9	51

* The contributions from graphs (1a) and (1b) are actually somewhat dependent on the detailed shape of the tensor potential. The contribution from graph (1a), however, is an integral over a function with a change in sign. The quantity ϕ which in Ref. 7) is similar to the function $C(K, k)$ in formula (19) of the present paper, changes its sign as K increases, and $a^{(a)}$ may become vanishingly small by a slight adjustment of the tensor force. On the contrary, $C(K, k)$ in $a^{(c)}$ has a fixed sign and $a^{(c)}$ is much less sensitive to the details of the tensor force. The contribution from (1b) involves an exchange and is usually smaller than one from (1a).

of graph (1c) is *not* negligible and could be of the same order of magnitude (with the proper sign) as the "experimental" value 57. However, we have not computed the contribution of graph (1d), because it would be an extremely tedious calculation.* Our main point is that there is at least one graph, (1c), the contribution of which can explain an appreciable part of the experimental spin-orbit splitting.

§ 5. The case of a hole in the closed shells

In the case of a hole in the closed shells, the second order graphs are represented on Fig. 3. These graphs are obtained from the corresponding ones in the

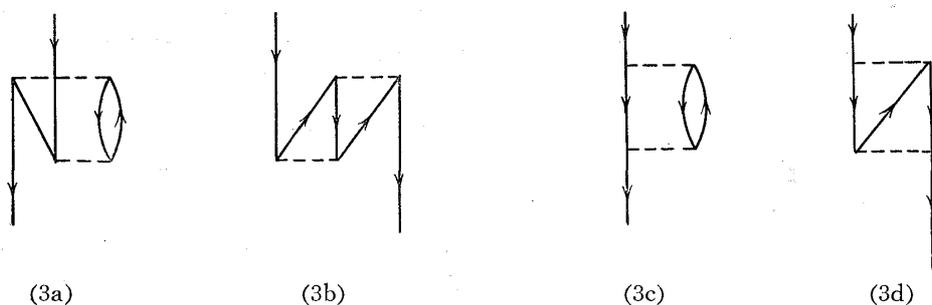


Fig. 3. The second-order graphs for hole.

particle case (Fig. 1) by replacing the incoming and outgoing particle lines by hole lines. For the bound states which are considered here, the particle is just above and the hole is just under the Fermi surface; in the limiting case of a large nucleus, the spacing between single particle levels goes to zero, and the particle and hole states become identical. It is therefore easy to see that the hole graphs of Fig. 3 give contributions which are just the opposite to those ones from the corresponding particle graphs of Fig. 1. The spin-orbit potential for one hole would therefore be $-a(1/r)(d\rho/dr)(\sigma \cdot \mathbf{l})$, with the same value of a as for one particle. The important contributions for a hole would now come from graphs (3c) and perhaps (3d), which are of the "reaction matrix" type.

The agreement with experiment is of the same kind as in the particle case. The experimental analysis which was quoted in § 4 involved also hole doublet splittings in Pb.²⁰⁷

§ 6. Conclusion

We can summarize the above discussion in the following way: The evaluation of the second order effect of the tensor forces, for the case of one particle outside the closed shells, first involves terms of the "reaction matrix" type, which describe collisions between the outside particle and one of the particles in the closed shells;

* This calculation could be very similar to the calculations of a_1 (graph (1b)) in I, and would be possible, in principle, for the case of a tensor force $r^2 \exp(-r^2/r_0^2)$.

these terms provide no appreciable spin-orbit effect. But there are also terms describing additional exclusion effects, which might be forgotten in a too naive extension of the Brueckner method to non-degenerate systems; those terms can explain, at least in part, the experimental spin-orbit splitting.

Those important exclusion effects may be described as the interdiction, for two nucleons of the closed shells, to jump by mutual excitation into an outer orbit which would already be occupied by another nucleon. This effect was here considered in the case of heavy nuclei. Similar calculations were carried out in the case of light nuclei. In that latter case, the important effective three-body vector forces which were derived by Feingold⁵⁾ from the tensor forces, or the exclusion effect of Terasawa⁶⁾ are of the same kind as the exclusion effect which was just described here. The smallness of the "reaction matrix" type graphs was also shown in light nuclei,^{5,6)} and even at all orders in heavy nuclei.¹⁰⁾

In the case of a hole in the closed shells, however, the important effect is of the "hole reaction matrix" type: the relevant intermediate states are those ones in which the hole is excited to some state of lower energy.

Turning again to the particle case, let us finally note that these exclusion effects (1c) and (1d) which appear to be important in the case of a bound outside particle would become negligible in the scattering problem for a particle of high energy, because the wave function of the closed shells would have little Fourier components in the state of the incident particle. Therefore, the exclusion mechanism, which provides a spin-orbit coupling for bound states, cannot account for the polarization of the high energy scattered nucleons. On the other hand, at high energy, the impulse approximation should be valid, and the nucleon-nucleus scattering problem is closely related to the two-body problem; the important effects therefore are of the "reaction", or rather "scattering matrix" type (Fig. 1a and 1b).^{*} If the low energy spin-orbit coupling is actually the result of exclusion type effects, the low and high energy spin-orbit couplings would result from quite different mechanisms, a result which is perhaps a little surprising and even unsatisfactory.

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^{*} At this two-body stage, there is still to be found the proper nucleon-nucleon potential. The problem of determining if this potential includes ^{1,2)} or not ³⁾ an elementary spin-orbit force does not seem to be uniquely set up at the present time.

Appendix

$C(K, k)$ is defined by

$$2\pi^2 k_0 C(K, k) = \int_{|\mathbf{K}-\mathbf{k}| < k_0} d\Omega_{\mathbf{K}} \frac{\mathbf{k} \cdot \mathbf{K}}{kK} \int_{\substack{|\mathbf{k}_s + \mathbf{K}| < k_0 \\ k_s > k_0}} \frac{d^3 \mathbf{k}_s}{(\mathbf{k} - \mathbf{k}_s) \cdot \mathbf{K} - K^2}, \quad (20)$$

where $\int d\Omega_{\mathbf{K}}$ denotes integration on \mathbf{K} angles. We consider only the case $k=k_0$. C is then found to be

$$\begin{aligned} C(K, k) &= (1/48) (K/k_0)^3 - (1/16) (K/k_0)^2 - (1/2) (K/k_0) + (13/12) \\ &+ [(1/64) (K/k_0)^3 - (1/8) (K/k_0) + (1/4) (k_0/K)] \log \left| \frac{2k_0 + K}{2k_0 - K} \right| \\ &+ [-(1/12) (K/k_0)^3 + (K/k_0) - (4/3)] \log 2. \end{aligned} \quad (21)$$

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