Matrix Elements between Nuclear Compound States and Dynamical Enhancement of the Weak Interaction

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A method to calculate the mean squared matrix element of the weak interaction between compound states is developed. The result is expressed in terms of matrix elements of the nucleon-nucleon strong and weak interactions times the Fermi distribution functions at finite temperature. Numerical calculations for ^{233}Th are in excellent agreement with recent measurements of parity nonconservation effects in neutron capture. In fact, our calculations prove that the factor of dynamical enhancement (ratio of compound-nucleus effect to single-particle one) really exceeds 100, thus making it unnecessary to assume a value of the weak constant bigger than standard one ($g \simeq 10^8\epsilon \sim 1$–$4$).

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The parity nonconserving (PNC) nucleon interaction in nuclei now attracts attention of both experimentalists and theorists, especially in connection with the recent experiments on slow neutron scattering through the compound nuclear states, where the measured PNC effect (dependence of cross section on neutron helicity) proved to be of order several percent [1,2] (cf. with the PNC effects in p-p or p-α scattering where effect is of order of 3×10^{-7}). Moreover, correlation of sign in the effect on close neutron resonances has been observed [2].

In the current literature [3–5], two different approaches to explain the great value of this effect coexist, based on different assumptions and contradicting each other. The first one, the statistical model of dynamical enhancement, was considered in Refs. [6,7]. (In fact, a large value of the effect was predicted in the 1980–1981 papers of Ref. [7].) Within this approach, the essential enhancement of the parity violating amplitude in neutron capture arises from the mixing of closely lying (within interval of several eV) compound nuclear levels of opposite parity, and statistical enhancement ($\sim \sqrt{N}$) of the weak matrix element between compound wave functions composed of $N \sim 3 \times 10^5$ many-particle configurations. The estimate of the magnitude of the effect was given in [3,4,7], based on the standard Hamiltonian of the weak interaction of nucleons in a nucleus,

$$\hat{W} = \frac{Gg}{2\sqrt{2}m}\{(\sigma\mathbf{p}), \rho\}, \quad \varepsilon = 1.0 \times 10^{-8} g, \qquad (1)$$

where $G = 10^{-5}m^{-2}$ is the Fermi constant, m is the nucleon mass, $\mathbf{p}$ and σ are the neutron momentum and its doubled spin correspondingly, while ρ is the nuclear density; the nucleon dimensionless constant $g_{p,n}$ (see, e.g., Ref. [8]) is of order unity (now the notation ε is widely used [5]).

The second approach, the so-called "valence mechanism" [9] (see also [10]), is based on the assumption that the weak amplitude admixing the s wave with the initial p wave is dominated by direct matrix elements of the PNC potential (1) between these states, so the effect is assumed to be of single-particle nature. The valence mechanism gives correlations of the sign in the effect on the different resonances but to explain the observed magnitude of the effect in this approach, one has to use a neutron constant in Eq. (1) at least 2 orders of magnitude larger than is predicted by theory (see Refs. [5,10]). Thus, the two mechanisms require a neutron weak interaction constant which differs by 2 orders of magnitude in the range 1–300. It becomes even more important in connection with the so-called "Tsinoev puzzle" [11] where the observed PNC effect is 10^3 times bigger than the theoretical estimate.

Staying within the framework of the first approach (dynamical enhancement) we present here a method to calculate the mean squared weak matrix element between s and p compound resonances, in the statistical model with account for nuclear structure and realistic residual nucleon interaction. We should note that the matrix element between compound states was considered earlier in Refs. [3,4]. However, these works use some hypotheses which are not easy to justify. In the work [3] a proportionality relation between the matrix elements of the weak and residual interaction was used. In the work [4] it was supposed that the matrix element between compound states is given by the same formula as the matrix element of the nucleon excitation from the ground state with only some minor modifications (occupation numbers and the optical potential depend on the temperature of the compound nucleus). In our approach we have not used these hypotheses, and our result looks different [e.g., it is not proportional to the square of the frequency of the time-dependent field ω^2 or T^2 ($\omega = 0$ for the weak interaction, and T is a temperature)]. Note that we do not discuss sign correlations in the present paper.

Calculation of the mean squared weak matrix element is based on the equivalence theorem of canonical and microcanonical ensembles for a system with a large number of degrees of freedom. Let us remember that the wave function of any compound state with angular momentum j and parity π may be expressed as follows:

$$|j^\pi) = \sum_\alpha C_\alpha |\alpha\rangle, \quad |\alpha\rangle = (a^\dagger b c^\dagger d e^\dagger \cdots)_{j^\pi}|0\rangle, \qquad (2)$$

through their components $|\alpha\rangle$ being many-particle excitations over the shell-model ground state $|0\rangle$ [we will denote them by simple Dirac brackets saving the notation $|\,)$ for compound wave functions; here and in what follows the notation $(\cdots)_{j^\pi}$ means the coupling of nucleon creators $a^\dagger$ and destructors a to total angular momentum j and parity π]. Among them, it is reasonable to separate explicitly the contribution of the "principal components", $|j^\pi)$), dominating normalization of the compound state, Eq. (2). The energies of these components must be within the interval $[E-\frac{\Gamma_{\rm spr}}{2}, E+\frac{\Gamma_{\rm spr}}{2}]$, where E is the energy of the compound state and $\Gamma_{\rm spr}$ is the spreading width of the component (typically, $\Gamma_{\rm spr}\sim 2$ MeV, Refs. [7,12]). These components (which contain several excited nucleons) can be composed by excitations of protons and neutrons only inside incomplete (valence) shells. Mean squared values of the coefficients $C(E_\alpha)$ can be described by the formulas (see, e.g., Ref. [12])

$$\overline{C^2(E_\alpha)}=\frac{1}{\overline{N}}\Delta(\Gamma_{\rm spr},E-E_\alpha),\qquad \overline{N}=\frac{\pi\Gamma_{\rm spr}}{2d},$$
$$\Delta(\Gamma_{\rm spr},E-E_\alpha)=\frac{\Gamma_{\rm spr}^2/4}{(E-E_\alpha)^2+\Gamma_{\rm spr}^2/4}, \tag{3}$$

where E_α is the energy of an arbitrary many-particle configuration), d is the averaged energy distance between the resonances, and $\overline{N}$ is the number of principal components. The Breit-Wigner-type factor Δ, describing cutting off of weights before states distanced in energy, may be treated as a "spread" δ function normalized to be of order unity for $|E-E_\alpha|\le\Gamma_{\rm spr}/2$ and with conventional limit $\Delta(\Gamma_{\rm spr},E-E_\alpha)\to\frac{\pi\Gamma_{\rm spr}}{2}\delta(E-E_\alpha)$ for $\Gamma_{\rm spr}\to 0$. Thus, the coefficients before the "principal" components $\tilde{C}_\alpha$ in (2) are governed by the microcanonical ensemble rule [7,12]. A very important point that should be borne in mind is that there are no single-particle states of opposite parity having the same angular momenta within the valence shells. Since the weak interaction [Eq. (1)] mixes only states of such type, it follows from the definition of "principal" components that the weak matrix element between two compound states of close energy is dominated by the weak transitions between "small" components of one resonance and "principal" ones of the second resonance, and vice versa (this was first mentioned by the authors of Ref. [9], see also [7]). Any transfer of one particle from the valence shell to another one gives a rise in excitation energy as large as $E_{sp}\sim 8$ MeV (which is much more than typical matrix elements of the residual interaction V) leading out a configuration from the microcanonical ensemble of "principal" components according to Eq. (3). Therefore, one can easily generate the appropriate set of "small" configurations by means of first-order perturbation theory in the residual strong interaction V. Thus, matrix elements of the weak interaction between compound states look like

$$(s|W|p)=\sum_\alpha\frac{((s|V|\alpha\rangle\langle\alpha|W|p))}{E-E_\alpha}+\sum_\beta\frac{((s|W|\beta\rangle\langle\beta|V|p))}{E-E_\beta}, \tag{4}$$

where $|\alpha\rangle$ and $|\beta\rangle$ are small components, and compound states $|s))$, $|p))$ contain only principal components. We stress that we do not need any "exotic" parts of the residual strong interaction here. Since $E-E_\alpha\sim 8$ MeV$\gg V$ (see above), only the dominating and well-known parts [13–15] of the two-nucleon interaction

$$V=\frac{1}{2}\sum_{ab,cd}a^\dagger bV_{ab,cd}c^\dagger d, \tag{5}$$

which will be specified below, are important in Eqs. (4) and (5). Here, our consideration is general and not even confined to nuclear systems.

The weak interaction [Eq. (1)] is a single-particle operator. This fact allows one to the include weak interaction into the mean nuclear field and transfer the perturbation theory expansion in the single-particle orbitals: $\tilde{\psi}_a=\psi_a+\sum_A\frac{\langle\psi_A|W|\psi_a\rangle}{\epsilon_a-\epsilon_A}\psi_A$, where ϵ_a and ϵ_A are the energies of the orbitals ψ_a and ψ_A (differing by their parities), the large Latin indices label the corresponding off-valence-shell states. Thus, we can express the result in terms of the residual interaction renormalized by the weak interaction [$\tilde{V}_{ab,cd}=V(\tilde{a}\tilde{b},\tilde{c}\tilde{d})$]:

$$\tilde{V}_{abcd}=\sum_A\frac{V_{Ab,cd}}{\epsilon_a-\epsilon_A}w_{aA}+\sum_B\frac{V_{aB,cd}}{\epsilon_b-\epsilon_B}w_{Bb}+\sum_C\frac{V_{ab,Cd}}{\epsilon_c-\epsilon_C}w_{cC}+\sum_D\frac{V_{ab,cD}}{\epsilon_d-\epsilon_D}w_{Dd}; \tag{6}$$

here $w_{aA}\equiv\langle\psi_A|W|\psi_a\rangle$. With these notations, to the first order in V, Eq. (4) can be read as follows: $(s|W|p)=((s|\tilde{V}|p))$. The advantage of using the effective two-particle PNC interaction $\tilde{V}$ is that the matrix elements between compound states are expressed through the matrix elements $\tilde{V}_{ab,cd}$ between valence shell single-particle states. Thus we avoid the necessity of explicitly considering the "small" components of the compound states which we believe cannot be described by the same spreading widths as the principal components [see Eq. (3)].

Consider now the mean squared value of this matrix element:

$$\overline{(p|W|s)(s|W|p)}=\overline{((p|\tilde{V}|s))((s|\tilde{V}|p))}=\sum_{\alpha\beta}\overline{C_\alpha C_\beta((p|\tilde{V}|\alpha\rangle\langle\beta|\tilde{V}|p))}=\sum_\alpha\frac{1}{\overline{N}}\Delta(\Gamma_{\rm spr},E-E_\alpha)\overline{((p|\tilde{V}|\alpha\rangle\langle\alpha|\tilde{V}|p))}. \tag{7}$$

Here, we have expanded the compound state $|s)$ in terms of the components (2) and made use of the statistical independence of the coefficients C_α [see Eqs. (2),(3), Refs. [5–7,12]]:

$$\overline{C_\alpha C_\beta} = \overline{C_\alpha^2}\delta_{\alpha\beta} = \delta_{\alpha\beta}\frac{1}{\overline{N}}\Delta(\Gamma_{\rm spr}, E - E_\alpha). \quad (8)$$

In the second quantization representation, summation over α in (7) is equivalent to summation over different components of the operator V in Eq. (5), i.e., the problem is reduced to the calculation of $((p|\tilde{V}\tilde{V}|p))$. Then, to calculate the averaging over p-resonance "principal" components $\overline{((p|\cdots|p))}$ in $\overline{W^2}$, let us use, instead of the present microcanonical ensemble, the equivalent canonical one (which may be chosen for a system with a large number of degrees of freedom by introducing the effective nuclear temperature T and chemical potentials λ_n, λ_p). In such a way, the expectation value in (8) is reduced to a canonical ensemble average with the standard contraction rules $((p|\overline{a^\dagger b}|p)) = \delta_{ab}\nu_a^T$, for ν_a^T being the finite temperature Fermi occupation probabilities, $\nu_a^T = \{\exp[(\epsilon_a - \lambda)/T] + 1\}^{-1}$. The canonical ensemble parameters T, λ_τ (τ means isospin projection) are to be determined from conventional "consistency" equations $E = \sum_a \nu_a\epsilon_a$, $Z = \sum_p \nu_p$, and $N = \sum_n \nu_n$ for the excitation energy E (being equal to the neutron separation energy, B_N), nuclear charge Z, and neutron number N correspondingly. After contraction evaluations one simply obtains from (7)

$$\sqrt{\overline{W^2}} = \sqrt{\frac{2d}{\pi\Gamma_{\rm spr}}}\left\{\sum_{abcd}\nu_a^T(1-\nu_b^T)\nu_c^T(1-\nu_d^T)\frac{1}{4}\mid \tilde{V}_{ab,cd} - \tilde{V}_{ad,cb}\mid^2 \Delta(\Gamma_{\rm spr}, \epsilon_a - \epsilon_b + \epsilon_c - \epsilon_d)\right\}^{\frac{1}{2}}. \quad (9)$$

The argument of the function Δ here is the change of the energy: $E - E_\alpha = \epsilon_a - \epsilon_b + \epsilon_c - \epsilon_d$, and $\tilde{V}$ is given by Eq. (6). In fact, it is an approximate energy conservation law with an accuracy up to the width of states.

The numerical calculations for ^{233}Th have been performed with the use of single-particle basis of states obtained by numerical calculations of the eigenvalue problem for the Woods-Saxon potential with spin-orbital interaction in the form $U(r) = -U_0 f(r) + U_{ls}(\sigma\mathbf{l})[\hbar/(m_\pi c)]^2\frac{1}{r}\frac{df}{dr} + U_C$ with $f(r) = (1 + \exp[(r - R)/a])^{-1}$, where $\mathbf{l}$ is the orbital angular momentum, U_C means Coulomb correction for protons, $U_C = 3Ze^2/(2R)[1 - r^2/(3R^2)]$, $r \le R$ and $U_C = Ze^2/r$, $r > R$, for R, a, and r being the nuclear radius, diffusity parameter, and radial variable correspondingly. The parameter values were used in accordance with Bohr-Mottelson formulas (see Ref. [12]) for the case of ^{233}Th: they are close to those established for heavy nuclei like lead (Ref. [15]) to reproduce single-particle properties. As for the residual interaction, we have employed the most widely used Landau-Migdal particle-hole interaction of contact type with spin- and isospin-exchange terms which rises to Landau Fermi liquid theory (Ref. [13]); for the case of a nucleus it was established in the theory of finite Fermi systems [14,15] by summation of all graphs irreducible in the particle-hole direction. In that case, the explicit form of the matrix V in (5) is given by the second quantized version of the interaction

$$V(\mathbf{r},\mathbf{r}') = C\delta(\mathbf{r} - \mathbf{r}')[f + f'\tau\tau' + g\sigma\sigma' + g'\tau\tau'\sigma\sigma'], \quad (10)$$

where $C = 300$ MeV fm^3 is the universal Migdal constant [14,15], σ (σ') and τ (τ') mean particle (hole) spin and isospin Pauli matrices, respectively, and the strengths f, f', g, g' are in fact functions of r via density dependence: $f = f_{\rm in} - (f_{\rm ex} - f_{\rm in})[\rho(r) - \rho(0)]/\rho(0)$ (the same for g, g') with ansatz $\rho(r) = \rho(0)f(r)$ (see above). (Quantities subscripted by "in" and "ex" characterize interaction strenghs in the depth of the nucleus and on its surface, respectively.) This interaction, with its parameter values listed below, has been successfully used by many authors (see Ref. [15]) to quantitatively describe a great amount of various properties of heavy nuclei. The value of temperature $T = 0.6$ MeV was used in accordance to the consistency condition for excitation energy (see above).

We present here the results for the conventional choice of values for parameters in the Landau-Migdal interaction, Eq. (10), which has been widely used for heavy nuclei (see [14,15] and references therein), namely, $f_{\rm ex} = -1.95$, $f_{\rm in} = -0.075$, $f'_{\rm ex} = 0.05$, $f'_{\rm in} = 0.675$, $g_{\rm in} = g_{\rm ex} = 0.575$, and $g'_{\rm in} = g'_{\rm ex} = 0.725$. Note that the exchange matrix elements of V enter in Eq. (9) but, generally, the values of the parameters f, f', g, and g' are chosen in such a way that the exchange terms are already included (it can always be done by use of the Firtz transformation). The variant referred to below as I corresponds to this standard procedure; we present also the results for the case when the exchange terms in (9) are included explicitly (referred to as II). The results for $\sqrt{\overline{W^2}}$ (8) may be expressed explicitly in terms of the proton and neutron weak constants g_p and g_n in the form

$$\sqrt{\overline{W^2}} = \frac{1}{\overline{N}}\sqrt{\overline{N}}\sqrt{(\Sigma_{pp}g_p)^2 + (\Sigma_{nn}g_n)^2 + \Sigma_{pn}g_pg_n}\ (\text{meV}); \quad (11)$$

the numerical calculation of the constants Σ gives the following results:

$$\text{I}: \quad \sqrt{\overline{W^2}} = 2.08\ \text{meV},$$

$$\text{II}: \quad \sqrt{\overline{W^2}} = 3.57\ \text{meV}.$$

The experimental value is $\sqrt{\overline{W^2}} = 1.39^{+0.55}_{-0.38}$ meV [2]. The values of $\sqrt{\overline{W^2}}$ for the cases I and II were obtained for the conventional choice of weak constants, $g_p = 4$ and $g_n = 1$ (Ref. [10]). (In the notation widely adopted in the current literature [2], for the neutron case it corresponds to the value $\varepsilon = 10^{-8}g_n = 10^{-8}$). Now, we can compare this result with single-particle (valence) estimation $w_{\rm val}$. In the valence mechanism, only single-particle components contribute (in ^{233}Th, $4s$ and $4p$ neutron states). Therefore, the valence model result is

$$w_{\rm val} \simeq \frac{1}{\overline{N}}\langle 4s|W|4p\rangle \simeq \frac{1}{\overline{N}} g_n 0.740 \text{ eV} = 1.72 \times 10^{-3} \text{ meV}. \quad (12)$$

Thus, the statistical contribution is 10^3 times bigger [due to the extra factor $\sqrt{\overline{N}}$, compare Eqs. (9) and (11) with (12)]. This factor reflects the incoherent contribution of all N components. Calculations fulfilled for other sets of parameters display no strong sensitivity of the numerical results to variations of both single-particle basis and residual interaction. Let us point out that in our approach the only essential assumption made is that of the statistical properties of the distribution for coefficients C_α in Eqs. (2),(8). As far as the uncertainty in definition of $\overline{N}^{-1/2}$ is concerned, two estimates for it, namely $\overline{N}^{-1/2} \simeq \sqrt{\frac{2d}{\pi\Gamma_{\rm spr}}}$ (for $d = 17$ eV in the ^{233}Th case and spreading $\Gamma_{\rm spr} \simeq 2$ MeV) and that from the widths of the compound resonances, $\overline{N}^{-1/2} \simeq \sqrt{\langle\Gamma_n/\Gamma_n^0\rangle}$, give approximately equal values $\overline{N}^{-1/2} \simeq 2.3 \times 10^{-3}$ with accuracy up to a factor of 2 [here Γ_n^0 is the width of the s or p single-particle resonance (see Ref. [12]), and Γ_n is the width of the s or p compound resonance correspondingly].

The results of this work can be summarized as follows. A consistent method to calculate the mean squared weak matrix element between two compound states of opposite parity is proposed, based on a statistical model with account for nuclear structure. The results prove that the dynamical enhancement $\sim \sqrt{\overline{N}}$ does really exist. The observed large value of this quantity for ^{233}Th is explained in terms of the model with the conventional neutron weak constant. Moreover, even for the zeroth value of the neutron constant the effect is still reproduced without substantial cutoff because of the proton PNC transitions in the nuclear compound state. (In fact, even for $g_n = 1$, the proton contribution is a few times larger due to the bigger value of constant g_p.) Further experiments in this region would be of great importance.

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