Chapter 7
Nuclear Level Calculation

The nuclear level P, CP-odd effects arise in the form of P, CP-odd nuclear moments, induced by P, CP-odd hadron level interactions. The leading P, CP-odd nuclear moment is of course the nuclear electric dipole moment (EDM), which enhances the contribution of P, CP-odd pion-nucleon interaction via many-body effects. The nuclear EDM is measurable in light nuclear systems such as the deuteron and the ^{3}He nucleus, with recent experimental developments using storage rings [1–4]. As the experimental prospects show a very high sensitivity of $O(10^{-29})e$ cm, it is of primary interest to evaluate the nuclear EDM for the deuteron and ^{3}He nucleus due to the P, CP-odd hadron level processes.

For atomic systems, the situation is different. There the nuclear EDM is actually screened by atomic electron rearrangement, and only a minor effect due to the finite size of the nucleus can contribute to the atomic EDM. This phenomenon first pointed by Schiff [5], leads to the suppression of the nuclear P, CP-odd effects in atoms. The relevant P, CP-odd nuclear moment for the atomic EDM is then the *nuclear Schiff moment*. In this discussion, we are also interested in the atomic EDMs of heavy nuclei where, in spite of the suppression due to Schiff's screening, the P, CP-odd hadronic effects are expected to be sufficiently enhanced via nuclear many-body physics.

To evaluate these P, CP-odd nuclear moments, the calculation of the nuclear wave functions are needed. As nuclei are made of protons and neutrons, the nuclear level calculation involves difficulties due to the many-body problem [7, 8]. For light nuclear systems, *ab initio* methods can be used. For heavy nuclei, however, the *ab initio* methods cannot be applied, due to the calculational cost increasing exponentially in nucleon number. For heavy nuclear systems of interest (^{129}Xe, ^{199}Hg, ^{211}Rn and ^{225}Ra), we will use the results from the sophisticated mean-field approach.

In this chapter, we will first see the *ab initio* calculations of the EDMs of light nuclei (deuteron and ^{3}He). We will then review in detail the screening of the P, CP-odd nuclear EDM in atomic system pointed by Schiff and the formula of the nuclear Schiff moment as important P, CP-odd mechanism contributing to the atomic EDM. We will next present the derivation of the leading P, CP-odd nuclear moments (the nuclear

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EDM, Schiff moment and magnetic quadrupole moment) for heavy nuclei within a simple model. After this simple calculation, a sophisticated mean-field approach is reviewed, and its results for the evaluation of the nuclear Schiff moments of heavy nuclei (^{129}Xe, ^{199}Hg, ^{211}Rn and ^{225}Ra) are presented. We finally summarize the nuclear level P, CP-odd moments for all nuclei relevant to the discussions in this chapter. Note that the electric charge e is defined as $e = |e| > 0$ in this chapter, in contrast to the previous chapters.

7.1 Ab Initio Calculations: Deuteron and ^{3}He EDM

Let us first present the *ab initio* calculations of the EDMs in the deuteron and the ^{3}He nucleus. The motivation for the study of these light nuclei is as follows. Recently, new experimental techniques of EDM measurements using magnetic storage ring are in preparation [1–4], and the EDM of light nuclei is the main focus. The EDM of light nuclei has the following advantages. The first advantage is that the system can be measured with high precision. The projected experiment of BNL is aimed at reaching the sensitivity of $O(10^{-29})e$ cm for the deuteron EDM. The second advantage is the absence of electrons which suppress the P, CP-odd nuclear effect through Schiff's screening phenomenon. These arguments indicate that the detection of EDMs in light nuclei has more significant sensitivity than the experiments on measuring hadron level P and CP violations. Although the small number of nucleons in the system, the EDM of light nuclei is actually a very competitive probe of new physics. Here we present the calculation of the deuteron EDM [6] and ^{3}He EDM [9].

The calculation of the deuteron EDM was first done by Khriplovich and Korkin with old strong potential [10]. A more complete analysis was made by Liu and Timmermans using three phenomenological nuclear potentials [6]: Argonne v_{18} [11], Nijmegen models Reid93 and Nijm II [12]. The dependence of the P, CP-odd pion-nucleon, ρ-meson-nucleon, η-meson-nucleon and ω-meson-nucleon interactions were studied. They found the dominance of the isovector pion-nucleon coupling for P, CP-odd interactions while all P, CP-odd hadronic interactions have similar magnitudes. The contribution to the deuteron EDM is composed of (a) single nucleon contribution ($d_A^{(Nedm)}$), (b) polarization contribution ($d_A^{(pol)}$), (c) contribution from exchanged current (in this thesis, we neglect its effect). In the case of the deuteron, the single nucleon contribution is simply given by the sum of proton and neutron EDMs ($d_d^{(Nedm)} = d_n + d_p$), since this is the allowed isoscalar combination. The polarization contribution is determined by the spin/isospin selection rules as

$$\begin{aligned} d_d^{(pol)} &= \sum_{i=1}^{A=2} \Big\langle \tilde{d} : j = 1, j_z = 1 \,\Big|\, e_i z_i \,\Big|\tilde{d} : j = 1, j_z = 1 \Big\rangle \\ &= \frac{e}{\sqrt{6}} \langle d || \mathbf{r} || d' \rangle \cdot \frac{1}{2} \langle I = 0 | \tau_1^z - \tau_2^z | I = 1, I_z = 0 \rangle = \frac{e}{\sqrt{6}} \langle d || \mathbf{r} || d' \rangle \end{aligned} \quad (7.1)$$

where $z \equiv z_1 - z_2$. Here $|\tilde{d} : j = 1, j_z = 1\rangle$ is the deuteron ground state wave function polarized in the z-axis, with $|d\rangle$ and $|d'\rangle$ its respective P, CP-even and P, CP-odd components. In the second line, we have factored out the isospin space, with the expression $\langle d||\mathbf{r}||d'\rangle$ denoting the reduced matrix element, and the second element is the matrix element of the isospin part with τ_1^z and τ_2^z the generator of the isospin $SU(2)$ group acting on the first and the second nucleons of the deuteron, respectively. The center of mass frame $\sum_i^A \mathbf{r}_i = 0$ was assumed. The wave functions $|d\rangle$ and $|d'\rangle$ were calculated by using the following P, CP-odd nucleon-nucleon (N-N) potential:

$$W(\mathbf{r}_a - \mathbf{r}_b) = -\frac{g_{\pi NN}}{8\pi m_p}\left[\left(\bar{g}^{(0)}_{\pi NN}\tau_a \cdot \tau_b + \bar{g}^{(2)}_{\pi NN}(\tau_a \cdot \tau_b - 3\tau_a^z \tau_b^z)\right)(\boldsymbol{\sigma}_a - \boldsymbol{\sigma}_b) + \bar{g}^{(1)}_{\pi NN}(\tau_a^z \boldsymbol{\sigma}_a - \tau_b^z \boldsymbol{\sigma}_b)\right] \cdot \nabla_a \frac{e^{-m_\pi r_{ab}}}{r_{ab}} \tag{7.2}$$

where a and b denote the indices of the two interacting nucleons, and $r_{ab} \equiv |\mathbf{r}_a - \mathbf{r}_b|$. The contribution from the exchanged current is suppressed compared to the polarization contribution with the P, CP-odd pion-nucleon couplings of the same order of magnitude [6]. If we neglect the contribution from ω, ρ and η-mesons and consider the pion exchange as the leading contribution, we obtain the following expression for the deuteron EDM:

$$d_d = d_n + d_p - 0.015 g_{\pi NN} \bar{g}^{(1)}_{\pi NN} \times 10^{-13} e\,\text{cm}. \tag{7.3}$$

The sign for isovector coupling was reversed from the result of Ref. [6] due to the difference of convention.

The calculation of the ^{3}He EDM was done by Stetcu et al. The ^{3}He EDM is also given by the single nucleon, polarization and exchanged current contributions. In this work, the exchanged current was neglected, following the small result of the deuteron EDM [6]. The single nucleon contribution is

$$d_{\text{He}}^{(Nedm)} = \langle \text{He}| \sum_{i=1}^{A=3} \frac{1}{2}\left[(d_p + d_n) + (d_p - d_n)\tau_i^z\right]\sigma_i^z |\text{He}\rangle \tag{7.4}$$

where $|\text{He}\rangle$ is the ground state of ^{3}He nucleus within the P and CP conserving hamiltonian. The contribution from the polarization can be written in the second order of perturbation as

$$\mathbf{d}_{\text{He}}^{(pol)} \approx \langle \text{He}| \sum_{i=1}^{A=3} \frac{e}{2}(1 + \tau_i^z)\mathbf{r}_i \sum_{n \neq 0} \frac{1}{E_0 - E_n} |n\rangle\langle n|W|\text{He}\rangle \tag{7.5}$$

where n are the opposite parity states, E_n their corresponding energy, and W the P, CP-odd interactions of Eq. (7.2).

The evaluation of the ^{3}He wave functions was done in the *ab initio* no-core shell model approach [13, 14] with truncated harmonic oscillator basis. The nuclear forces used in the calculation are the Argonne $v18$ [11], the nonlocal Bonn [15] potentials, with Coulomb interaction and isospin violation taken into account, and two-, three-body interactions derived from EFT [16–19].

The calculation of the dependence of the EDM of the ^{3}He nucleus on P, CP-odd pion-nucleon couplings gives the following result [9]:

$$d_{\rm He} = g_{\pi NN}\left(-0.015\bar{g}^{(0)}_{\pi NN} - 0.023\bar{g}^{(1)}_{\pi NN} + 0.036\bar{g}^{(2)}_{\pi NN}\right) \times 10^{-13} e\,{\rm cm} - 0.04 d_p + 0.90 d_n \tag{7.6}$$

where we have not explicitly added the contribution of the P, CP-odd pion-nucleon interactions coming from the single nucleon EDM (pion-loop contribution). Here again, the sign for isoscalar and isovector couplings was reversed from the result of Ref. [9] due to the difference of convention. This result shows that the ^{3}He EDM has higher sensitivity than the deuteron and nucleon EDMs to the P, CP-odd pion-nucleon interactions. All measurements of EDMs of nucleon, deuteron and ^{3}He are complementary.

7.2 Schiff's Screening Phenomenon and the Nuclear Schiff Moment

We now move to the evaluation of nuclear P and CP violations for heavy nuclei in atoms, where nuclear EDM is shielded by atomic electrons. The screening phenomenon of the intrinsic EDM of components in atomic system was first shown by Schiff [5]. Actually, the theorem of Schiff states that the EDM of non-relativistic point-like particle in a neutral electrostatically bound system is completely shielded. The effect of the nuclear EDM in atomic systems is therefore suppressed. Schematically, the screening of the nuclear EDM can be described as shown in Fig. 7.1.

Let us see this phenomenon in detail. The atomic EDM receives contribution from the sum of the intrinsic EDMs of its components, and the polarization of the system induced by the mixing of opposite parity states due to P, CP-odd interactions ($\langle s_{1/2}|H_{\not P \not T}|p_{1/2}\rangle$). The atomic EDM (and more generally the EDM of neutral electrostatically bound systems) can then be expressed as

$$\mathbf{d}_{\rm atom} = \sum_i \langle \Psi | d_i \gamma_0 \boldsymbol{\sigma}_i | \Psi \rangle + 2 \sum_M \sum_i \frac{\langle \Psi | Q_i e \mathbf{r}_i | M \rangle \langle M | H_{\not P \not T} | \Psi \rangle}{E_0 - E_M} \tag{7.7}$$

where the first term refers to the sum of the intrinsic EDMs of the components and the second term to the contribution of the polarization arising from P, CP-odd interactions. Ψ is the atomic state of interest, unperturbed by P, CP-odd interactions,

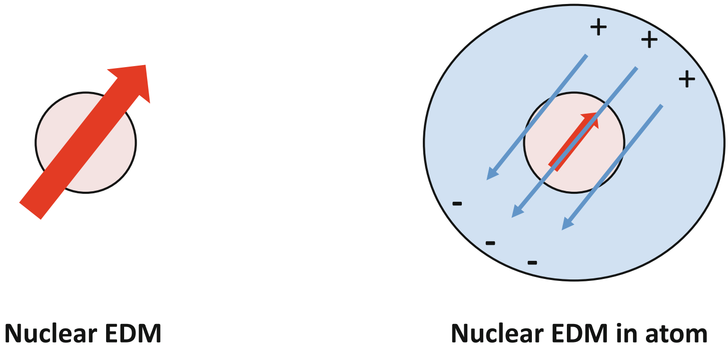

Fig. 7.1 Schematic representations of the bare nuclear EDM (*left side*) and the nuclear EDM screened in atom (*right side*). The effect of nuclear EDM is suppressed by the internal rearrangement of the atomic systems

d_i the intrinsic EDM of the atomic components (electrons and nucleus), Q_i and $\mathbf{r}_i$ are the charges and coordinates of each component, M the intermediate atomic states (with opposite parity against $|\Psi\rangle$) and $H_{\not P \not T}$ the P, CP-odd interaction. γ_0 and $\boldsymbol{\sigma}_i \equiv \gamma_0 \gamma_5 \boldsymbol{\gamma}_i$ are Dirac matrices acting independently on each component labeled by i.

The contribution from the first term, i.e. the sum of the EDMs of components can be splitted into the non-relativistic and relativistic parts. Here we write down its hamiltonian:

$$H_{\rm comp} = -\sum_i d_i \gamma_0 \boldsymbol{\sigma}_i \cdot \mathbf{E}_{\rm ext} = -\sum_i d_i \boldsymbol{\sigma}_i \cdot \mathbf{E}_{\rm ext} - \sum_i d_i (\gamma_0 - 1) \boldsymbol{\sigma}_i \cdot \mathbf{E}_{\rm ext} \quad (7.8)$$

where $\mathbf{E}_{\rm ext}$ is the external electric field acting on the component EDMs. We will now see that the non-relativistic contribution (first term) will be cancelled by the polarization contribution. The EDMs of the components interact with the internal electric field, thus generating mixing between opposite parity states. The corresponding (non-relativistic) EDM interaction which polarizes the system can be written as

$$H_{\not P \not T} = -\sum_i \mathbf{d}_i \cdot \mathbf{E}_{\rm int} = \sum_i \frac{1}{Q_i e} \mathbf{d}_i \cdot \nabla_i U(\mathbf{r}) = i \sum_i \frac{1}{Q_i e} [\mathbf{p}_i, H_0] \cdot \mathbf{d}_i \ . \quad (7.9)$$

where $\mathbf{d}_i \equiv d_i \boldsymbol{\sigma}_i$. U and H_0 are respectively the potential energy and the P, CP-even hamiltonian of the atomic system. This equation states that the charge of the system will be polarized proportional to EDMs of components. The contribution from the polarization is then

$$|\Psi'\rangle = |\Psi\rangle + \sum_m \frac{|m\rangle\langle m| H_{\not P \not T} |\Psi\rangle}{E_0 - E_m} = \left(1 + i \sum_i \frac{1}{Q_i e} \mathbf{d}_i \cdot \mathbf{p}_i \right) |\Psi\rangle \ . \quad (7.10)$$

The EDM induced by intrinsic electron EDM is then

$$\begin{aligned}\langle \Psi' | \sum_i Q_i e \mathbf{r}_i | \Psi' \rangle &= \langle \Psi | \left(1 - i \sum_k \frac{1}{Q_k e} \mathbf{d}_k \cdot \mathbf{p}_k \right) \sum_i Q_i e \mathbf{r}_i \left(1 + i \sum_j \frac{1}{Q_j e} \mathbf{d}_j \cdot \mathbf{p}_j \right) | \Psi \rangle \\ &= \langle \Psi | \, i \left[\sum_l Q_i e \mathbf{r}_i, \sum_k \frac{1}{Q_k e} \mathbf{d}_k \cdot \mathbf{p}_k \right] | \Psi \rangle \\ &= - \langle \Psi | \sum_i \mathbf{d}_i \, | \Psi \rangle \, . \end{aligned} \tag{7.11}$$

We see that the polarization of the system completely cancels the direct contribution given by the sum of EDMs of *non-relativistic* constituents with intrinsic EDM. This cancellation of the non-relativistic EDM contribution by the internal rearrangement is called the Schiff's theorem [5]. This conclusion is very important since the EDM of the nucleus which can be treated as non-relativistic in atomic systems is shielded, so that its effect is largely suppressed. We should also emphasize that the above cancellation applies only for the non-relativistic contribution of the EDM of the constituents. The EDM of relativistic particles actually gives an additional contribution to the polarization of the atomic system (additional effective interaction to $H_{\not P \not T}$), which is not cancelled by the direct contribution. The P, CP-odd electron-nucleon interactions also contribute to the atomic polarization (with no direct contribution), thus giving a non-vanishing EDM to the atom. The effects of relativistic electrons and P, CP-odd electron-nucleon interactions are discussed in the next chapter.

Let us see Schiff's screening phenomenon in the atomic system with a finite size nucleus having an EDM [5, 20]. The hamiltonian of the neutral atomic system with Z electrons is given by

$$H = \sum_{i=1}^{Z} \left[K_i - \int \frac{e^2 \rho(\mathbf{r}) d^3 r}{|\mathbf{R}_i - \mathbf{r}|} - e \mathbf{R}_i \cdot \mathbf{E}_{\text{ext}} \right] + \sum_{i>k}^{Z} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_k|} - \mathbf{d}_A \cdot \mathbf{E}_{\text{ext}} \tag{7.12}$$

where K_i and R_i are the kinetic energy and the coordinate of the atomic electrons, respectively, and the nuclear charge density $\rho(\mathbf{r})$ is normalized with $\int \rho(\mathbf{r}) d^3 r = Z$. The nuclear EDM is given by $\mathbf{d}_A \equiv \int e \mathbf{r} \rho(\mathbf{r}) d^3 r$. Let us now add to this hamiltonian the following additional auxiliary term

$$V_{pol} = \mathbf{d}_A \cdot \mathbf{E}_{\text{ext}} - \frac{1}{eZ} \sum_{i=1}^{Z} \mathbf{d}_A \nabla_i \int \frac{e \rho(\mathbf{r}) d^3 r}{|\mathbf{R}_i - \mathbf{r}|} \tag{7.13}$$

with $\nabla_i \equiv \partial / \partial R_i$. This new interaction can be expressed by the following commutation relation

$$\frac{i}{Zem_e} \sum_{i=1}^{Z} [\, \mathbf{p}_i, H \,] \cdot \mathbf{d}_A = \mathbf{d}_A \cdot \mathbf{E}_{\text{ext}} - \frac{1}{eZ} \sum_{i=1}^{Z} \mathbf{d}_A \nabla_i \int \frac{e \rho(\mathbf{r}) d^3 r}{|\mathbf{R}_i - \mathbf{r}|} = V_{pol} \tag{7.14}$$

where we have used the fact that the total electron momentum $\sum_i \mathbf{p}_i$ commutes with the Coulomb interaction between electrons $\sum_{i>k}^{Z} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_k|}$. The addition of this auxiliary term does not affect the observation in the linear approximation in d_A, since $\langle \Psi | [\, \mathbf{p}_i , H \,] | \Psi \rangle \sim (E_0 - E_0) = 0$. This term is just the effective interaction given by the polarization of the atomic system. We thus obtain the following total hamiltonian shifted by V_{pol}:

$$\tilde{H} = H + V_{pol} = \sum_{i=1}^{Z} [K_i - e\varphi(\mathbf{R}_i) - e\mathbf{R}_i \cdot \mathbf{E}_{\text{ext}}] + \sum_{i>k}^{Z} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_k|} \tag{7.15}$$

with the electrostatic potential given by

$$\varphi(\mathbf{R}) = \int \frac{e\rho(\mathbf{r})}{|\mathbf{R} - \mathbf{r}\,|} d^3r + \frac{1}{Z}(\mathbf{d}_A \cdot \nabla) \int \frac{\rho(\mathbf{r})}{|\mathbf{R} - \mathbf{r}\,|} d^3r \, . \tag{7.16}$$

It is interesting to observe that Eq. (7.15) does not depend on the direct interaction between the nuclear EDM and the external electric field $\mathbf{E}_{\text{ext}}$. This is the screening phenomenon pointed by Schiff [5].

Let us expand the nuclear potential in r/R (multipole expansion). To the first order in r/R, the nuclear electrostatic potential of Eq. (7.16) can be written as

$$-\int e\rho(\mathbf{r}) \left(\mathbf{r} \cdot \nabla \frac{1}{R}\right) d^3r + \frac{1}{Z} (\mathbf{d}_A \cdot \nabla) \frac{1}{R} \int \rho(\mathbf{r}) d^3r = 0 \, . \tag{7.17}$$

This cancellation means that the EDM of the nucleus is totally screened if the nucleus is point-like. This is also the consequence of Schiff's screening phenomenon. The shielding of the nuclear EDM contribution is however not complete if we take the finite size of the nucleus into account. This fact manifests itself through the electrostatic potential of the nucleus by the non-zero contribution of the third order terms in r/R:

$$\varphi^{(3)} = -\frac{1}{6} \int e\rho(\mathbf{r}) r_i r_j r_k d^3r \nabla_i \nabla_j \nabla_k \frac{1}{R} + \frac{1}{2Z} (\mathbf{d}_A \cdot \nabla) \nabla_i \nabla_j \frac{1}{R} \int \rho(\mathbf{r}) r_i r_j d^3r \, . \tag{7.18}$$

Tensors $r_i r_j r_k$ and $r_i r_j$ are reducible, and their decompositions can be written as follows:

$$r_i r_j r_k = \left[r_i r_j r_k - \frac{1}{5} r^2 (r_i \delta_{jk} + r_j \delta_{ik} + r_k \delta_{ij}) \right] + \frac{1}{5} r^2 (r_i \delta_{jk} + r_j \delta_{ik} + r_k \delta_{ij}) \tag{7.19}$$

$$r_i r_j = \left[r_i r_j - \frac{1}{3} r^2 \delta_{ij} \right] + \frac{1}{3} r^2 \delta_{ij} . \tag{7.20}$$

It is thus possible to decompose the third order $\varphi^{(3)}$ to the rank-3 octupole potential [first terms of Eqs. (7.19) and (7.20)] and the rank-1 "Schiff" potential [second terms of Eqs. (7.19) and (7.20)]. The electric octupole moment is a P, CP-odd moment, so it can contribute to the atomic EDM through higher nuclear spin state. In this discussion, the nuclear states in question are spin 1/2 states, so we omit the octupole potential. By subtituting the first term of Eqs. (7.19) and (7.20) to Eq. (7.18), we obtain the following rank-1 Schiff potential:

$$\varphi_{\text{Schiff}} = -\mathbf{S}_A \cdot \nabla \left(\nabla^2 \frac{1}{R} \right) = 4\pi \mathbf{S}_A \cdot \nabla \delta^3(\mathbf{R}) \tag{7.21}$$

where $\mathbf{S}_A$ is defined as

$$\mathbf{S}_A \equiv \frac{1}{10} \left[\int e\rho(\mathbf{r})\mathbf{r}r^2 d^3r - \frac{5}{3}\mathbf{d}_A \frac{1}{Z} \int \rho(\mathbf{r}) r^2 d^3r \right] . \tag{7.22}$$

This is the *nuclear Schiff moment*. The Schiff moment operator is thus written as

$$\hat{\mathbf{S}} = \frac{1}{10} \sum_{p=1}^{Z} e \left(r_p^2 - \frac{5}{3} \langle r^2 \rangle_{\text{ch}} \right) \mathbf{r}_p \tag{7.23}$$

where $\langle r^2 \rangle_{\text{ch}} \equiv \frac{1}{Z} \int r^2 \rho(\mathbf{r}) d^3r$ is the average (squared) charge radius of the nucleus, and $\mathbf{r}_p$ the coordinate operator of the nuclear proton. The above Schiff moment operator satisfies $\mathbf{S}_A = \langle \Psi_A | \hat{\mathbf{S}} | \Psi_A \rangle$ with Ψ_A the nuclear state vector. Note that the Schiff potential (7.21) acts on the atomic electron states, whereas the Schiff operator (7.23) operates in the nuclear space. If we consider also the charge distribution of the nucleons, we have to extend this expression to

$$\hat{\mathbf{S}} = \frac{1}{10} \sum_{N=1}^{A} \sum_{i_N} e_{i_N} \left[(\mathbf{r}_N + \boldsymbol{\rho}_{i_N})^2 - \frac{5}{3} \langle r^2 \rangle_{\text{ch}} \right] (\mathbf{r}_N + \rho_{i_N}) \tag{7.24}$$

where N denotes the index of each nucleon and i_N the index of the charged constituents inside the Nth nucleon. The coordinate of the i_Nth constituent relative to the center of mass of the Nth nucleon $\mathbf{r}_N$ is given by $\boldsymbol{\rho}_{i_N}$, so that the intrinsic EDM of the nucleon N can be written as $\mathbf{d}_N = \sum_{i_N} e_{i_N} \boldsymbol{\rho}_{i_N}$. The charge distribution inside the nucleon is smaller than the size of the nucleus, so taking only up to the first order in ρ_{i_N}, we obtain the following final formula for the nuclear Schiff moment

$$\hat{\mathbf{S}} = \hat{\mathbf{S}}^{\text{ch}} + \hat{\mathbf{S}}^{\text{nucleon}} \tag{7.25}$$

where

$$\hat{\mathbf{S}}^{\rm ch} = \frac{e}{10}\sum_{p=1}^{Z}\left(r_p^2 - \frac{5}{3}\langle r^2\rangle_{\rm ch}\right)\mathbf{r}_p \tag{7.26}$$

$$\hat{\mathbf{S}}^{\rm nucleon} \approx \sum_{N=1}^{A}\left\{\frac{1}{6}\left(r_N^2 - \langle r^2\rangle_{\rm ch}\right)\mathbf{d}_N + \frac{1}{5}\left((\mathbf{r}_N\cdot\mathbf{d}_N)\mathbf{r}_N - \frac{r_N^2}{3}\mathbf{d}_N\right)\right\}. \tag{7.27}$$

The derivation of the above relations from Eq. (7.24) is given in Appendix F.

7.3 Derivation of P, CP-odd Nuclear Moments in a Simple Model

We will now try to derive the P, CP-odd nuclear moments of heavy nuclei in a simple model to see their qualitative properties. The P, CP-odd nuclear moments of interest are the nuclear EDM, the Schiff moment and the magnetic quadrupole moment, which give the leading contribution to nuclear and atomic P and CP violations. The derivation presented in this section follows the discussion of Ref. [21]. P, CP-odd nuclear moments are generated in the presence of P, CP-odd nucleon-nucleon (N-N) interactions. Let us assume the following P, CP-odd interaction:

$$W_{ab} = \frac{G_F}{\sqrt{2}}\frac{1}{2m_N}\{(\eta_{ab}\boldsymbol{\sigma}_a - \eta_{ba}\boldsymbol{\sigma}_b)\cdot\nabla\delta(\mathbf{r_a}-\mathbf{r_b}) \\ +\eta'_{ab}(\boldsymbol{\sigma}_a\times\boldsymbol{\sigma}_b)\cdot[(\mathbf{p}_a-\mathbf{p}_b)\delta(\mathbf{r}_a-\mathbf{r}_b)+\delta(\mathbf{r}_a-\mathbf{r}_b)(\mathbf{p}_a-\mathbf{p}_b)]\} \tag{7.28}$$

where a and b label nucleons in the nuclear system. η_{ab} and η'_{ab} are the P, CP-odd N-N coupling constants. This interaction is the non-relativistic approximation of the general contact P, CP-odd N-N interaction at the lowest order in derivatives. The relation between the scalar-pseudoscalar type P, CP-odd N-N couplings η_{ab} and the P, CP-odd pion-nucleon couplings of Eq. (6.3) is roughly $\eta_{ab} \sim O\left(\frac{\bar{g}_{\pi NN}g_{\pi NN}}{m_\pi^2 G_F/\sqrt{2}}\right) \sim O(10^7\bar{g}_{\pi NN})$ ($\bar{g}_{\pi NN}$ denotes $\bar{g}^{(0)}_{\pi NN}$, $\bar{g}^{(1)}_{\pi NN}$ and $\bar{g}^{(2)}_{\pi NN}$).

It is known that the nuclear interaction has strong pairing force, which pairs even number of nuclei, so that odd nuclei have one valence nucleon. By assuming the simple shell model (works for stable spherical nuclei with nucleon number $A \geq 20$), the valence nucleon feels the following P, CP-odd nuclear potential:

$$W = \frac{G_F}{\sqrt{2}}\frac{\eta_a}{2m_N}\boldsymbol{\sigma}\cdot\nabla\rho_A(r), \tag{7.29}$$

with $\eta_a \equiv \frac{Z}{A}\eta_{ap} + \frac{N}{A}\eta_{an}$, and $\rho_A(r)$ the density of nucleon inside the nucleus normalized with $\int\rho_A(r)d^3r = A$ (note that the definition of ρ and ρ_A are different!). The tensor type P, CP-odd N-N interaction [second term of Eq. (7.28)] does not contribute to the nucleus with one valence nucleon since nucleons in the core are paired to have zero angular momentum. We see from Eq. (7.29) that in this model the nuclear P, CP-odd effect occurs at the surface, so it grows slower than the total nucleon number A of the system.

It is known that the nuclear potential which is felt by valence nucleon and the nuclear density have the same shape. Their relation is then

$$\rho_A(r) = \frac{\rho_A(0)}{U(0)} U(r) \tag{7.30}$$

where $\rho_A(0)$ and $U(0) \sim -45$ MeV are the nuclear density and potential at the center of the nucleus, respectively. The potential felt by the valence nucleon can therefore be rewritten as

$$\tilde{U}(r) = U(r) + W(r) \approx U(|\mathbf{r} + \xi \boldsymbol{\sigma}|), \tag{7.31}$$

where $\xi \equiv \frac{G_F}{\sqrt{2}} \frac{\eta_a}{2m_N} \frac{\rho_A(0)}{U(0)}$. The wave function in this potential then becomes

$$\tilde{\Psi}(\mathbf{r}) = \Psi(\mathbf{r} + \xi \boldsymbol{\sigma}) = (1 + \xi \boldsymbol{\sigma} \cdot \nabla) \Psi(\mathbf{r}). \tag{7.32}$$

Following Refs. [8, 21], we obtain the next three formulae for the dependence of the nuclear EDM, Schiff moment and magnetic quadrupole moment, respectively, on the P, CP-odd N-N interactions:

$$d_A(\xi) = -e\xi \left(q - \frac{Z}{A} \right) t_j \tag{7.33}$$

$$S_A(\xi) = -\frac{eq}{2} \xi \left[\frac{1}{5} \left(t_j + \frac{1}{j+1} \right) r_{ex}^2 - \frac{1}{3} t_j \langle r^2 \rangle_{\mathrm{ch}} \right] \tag{7.34}$$

$$M_A(\xi) = \frac{e}{m_N} \xi \cdot (\mu - q)(2j - 1) t_j \tag{7.35}$$

where μ is the magnetic moment of the nucleus, $r_{ex}^2 \equiv \int r^2 |\tilde{\Psi}(\mathbf{r})|^2 d^3r$ is the mean square radius of the valence nucleon and $\langle r^2 \rangle_{\mathrm{ch}} \equiv \frac{1}{Z} \int r^2 \rho(\mathbf{r}) d^3r$ the mean square radius of the nuclear charge (with $\rho(\mathbf{r})$ the nuclear charge density). The coefficient q is the charge of the valence nucleon in unit of e ($q = 0$ when the valence nucleon is a neutron, and $q = 1$ for the proton). Here $t_j = 1$ is for a nucleus with $j = l + 1/2$, and $t_j = -\frac{j}{j+1}$ for a $j = l - 1/2$ nucleus. The derivation of the nuclear EDM and the Schiff moment in this simple model is presented in Appendix F.

The above estimation within a simple model gives us important qualitative information on the CP-odd nuclear moments. From the formula (7.34), we see that nuclei with valence neutron (^{129}Xe, ^{199}Hg, ^{211}Rn and ^{225}Ra) have no Schiff moment due to the overall factor $q = 0$. This means that P, CP-odd interactions between the valence neutron and the core cannot directly generate the nuclear Schiff moment. Moreover, in Ref. [8], it is assumed that the mean square radii of the valence nucleon and the nuclear charge are approximately equal ($r_{ex}^2 = \langle r^2 \rangle_{\mathrm{ch}} = \frac{3}{5} A^{2/3} r_0^2$). In this approximation, the nuclear Schiff moment of spin 1/2 s-wave nuclei vanishes. This is the case for ^{205}Tl nucleus. To do more quantitative analysis, more accurate determinations of r_{ex}^2 and $\langle r^2 \rangle_{\rm ch}$ are needed, and these are the subject of the next work. In our discussion, we will take the nuclear Schiff moment of ^{205}Tl to be zero. The magnetic quadrupole moment is not relevant to our discussion, since we are considering nuclei with spin 1/2.

Since we are interested in the EDM of heavy atoms, the EDM of heavy nuclei are also not relevant to our discussion, but here we should add some comments on the nuclear enhancement of P, CP-odd effect compared with the single nucleon EDM. The P, CP-odd N-N coupling generated from isoscalar P, CP-odd pion-nucleon interaction is $\frac{G_F}{\sqrt{2}}\eta_a \sim \frac{g_{\pi NN}\bar{g}^{(0)}_{\pi NN}}{m_\pi^2}$. Comparing with the contribution of the isoscalar P, CP-odd pion-nucleon interaction to the the single nucleon EDM $d_N(\bar{g}^{(0)}_{\pi NN}) \sim \frac{e g_{\pi NN}\bar{g}^{(0)}_{\pi NN}}{4\pi^2 m_N} \ln \frac{m_N}{m_\pi}$ [see Eq. (6.46)], the enhancement of the nuclear EDM against the single nucleon EDM is

$$\frac{d_A}{d_N} \sim \left| \frac{e\xi}{d_N} \right| \sim \left| \frac{3\pi}{2 m_\pi^2 r_0^3 U(0) \ln(m_N/m_\pi)} \right| \sim 12 \tag{7.36}$$

where we have assumed $1/\rho_A(0) = \frac{4}{3}\pi r_0^3$ with the internucleon distance $r_0 \sim 1.2$ fm, which is valid for nuclei of interest. We see that the nuclear EDM is sensitive on the P, CP-odd pion-nucleon couplings than the single nucleon EDM by more than one order of magnitude in this simple estimation. The nuclear enhancement is of course dependent on the model of CP violation at the hadron level. For the standard model contribution (see Chap. 9), the enhancement factor can be as large as 60 [24, 25]. We can thus expect a very good improvement of sensitivity against the CP violation of new physics with the progress of experimental studies of the nuclear EDM.

We should also give the dependence of the P, CP-odd nuclear moments on the EDM of the valence nucleon. With the same model assumptions, Ref. [21] (also Ref. [8]) gives the following formulae for the nucleon EDM dependence of the nuclear EDM, Schiff moment and magnetic quadrupole moment:

$$d_A(d_N) = d_N\, t_j \tag{7.37}$$

$$S_A(d_N) = \frac{d_N}{2}\left[\frac{1}{5}\left(t_j + \frac{1}{j+1}\right) r_{ex}^2 - \frac{1}{3} t_j \langle r^2 \rangle_{\rm ch}\right] \tag{7.38}$$

$$M_A(d_N) = \frac{d_N}{m_N}(2j-1) t_j \tag{7.39}$$

where d_N is the EDM of the valence nucleon. The derivation of the nuclear EDM and the Schiff moment is presented in Appendix F. The relations (7.38) and (7.39) have similar form as Eqs. (7.34) and (7.35). This implies again that the nuclear Schiff moment of the spin 1/2 s-wave nuclei is suppressed. This is the case for ^{205}Tl, ^{129}Xe and ^{225}Ra nuclei.

Phenomenologically, the valence nucleon is a superposition of the proton and neutron due to the configuration mixing. The mixing coefficients $\langle \sigma_p \rangle_z$ and $\langle \sigma_n \rangle_z$ can be obtained using the magnetic moment of the nucleus as follows:

$$\begin{cases} \mu_A = \mu_p \langle \sigma_p \rangle_z + \mu_n \langle \sigma_n \rangle_z \\ \langle \Psi : j, j_z = j \,|\, \sigma_z \,|\, \Psi : j, j_z = j \rangle = \langle \sigma_n \rangle_z + \langle \sigma_p \rangle_z \end{cases} \tag{7.40}$$

where μ_A is the nuclear magnetic moment (in unit of the Bohr magneton). Here the matrix element $\langle \Psi : j, j_z = j \,|\, \sigma_z \,|\, \Psi : j, j_z = j \rangle$ is 1 for $j = l + \frac{1}{2}$ nuclei, and $-\frac{j}{j+1}$ for $j = l - \frac{1}{2}$ nuclei (the same matrix element is needed for the derivation of the nuclear EDM generated by the valence nucleon EDM. The detail is given in Appendix F). The magnetic moment of the proton is $\mu_p = +2.7928$ and that of the neutron is $\mu_n = -1.9130$. The mixing coefficients $\langle \sigma_p \rangle_z$ and $\langle \sigma_n \rangle_z$ are needed to separate the EDM contribution of the valence proton and neutron, but also for the P, CP-odd electron-nucleon interactions, which will be reviewed in the next chapter.

In this section, we have seen that the Schiff moment of nuclei with valence neutron has no dependence on the P, CP-odd N-N interaction in the simple shell model. However, for heavy nuclei such as ^{129}Xe, ^{199}Hg, ^{211}Rn and ^{225}Ra nuclei, the whole nuclear system may be polarized by the P, CP-odd N-N interaction. This effect can be calculated with many-body methods using the *mean-field theory*, which will be reviewed in the next section. We must finally note that we have only *assumed* that the shell model works for odd nuclei in question. We have also assumed that nuclei are spherical. Deformed nuclei can enhance P, CP-odd moments with their close opposite parity levels. In the next section, we will review the calculational methods based on mean-field theory to treat the core polarization of heavy nuclei with valence neutron, and their results.

7.4 Evaluation of the ^{129}Xe, ^{199}Hg, ^{211}Rn and ^{225}Ra Nuclear Schiff Moments within Mean-Field Approach

Let us now present more sophisticated calculations of the nuclear wave functions needed to obtain the nuclear Schiff moment from core polarization. Ideally, the nuclear wave function should be obtained via some *ab initio* calculations, but this task is too difficult as the computational cost for solving the many-body problem increases exponentially with nucleon number. We must therefore introduce some approximations.

In many-body calculations, we often use the *Hartree-Fock method*. In the many-body system, the interaction between particles can be renormalized to a mean-field potential with residual interactions, which will be determined phenomenologically. With this approximation, the many-body calculation is thus reduced to an one-body problem (one-particle interacting with the mean field). The hamiltonian of the N-body system in the Hartree-Fock approximation can be written in the following form

$$H = H_0 + V^{N-1} \tag{7.41}$$

where H_0 is the hamiltonian of the single particle (kinetic terms + mean-field potential), and $V^{N-1} \equiv V_{\text{dir}} + V_{\text{ex}}$ is the Hartree-Fock potential, which satisfies the following relations:

$$V_{\text{dir}}(\mathbf{r})\Psi(\mathbf{r}) = \sum_{n=1}^{N-1} \int \Psi_n^\dagger(\mathbf{r}_1)\Psi_n(\mathbf{r}_1)V(\mathbf{r}_1,\mathbf{r})d^3r_1\,\Psi(\mathbf{r})$$

$$V_{\text{ex}}(\mathbf{r})\Psi(\mathbf{r}) = -\sum_{n=1}^{N-1} \int \Psi_n^\dagger(\mathbf{r}_1)\Psi(\mathbf{r}_1)V(\mathbf{r}_1,\mathbf{r})d^3r_1\,\Psi_n(\mathbf{r})\,. \tag{7.42}$$

These contributions can be illustrated diagramatically in Fig. 7.2.

Solving the Schrödinger equation for H is equivalent to solving the self-consistent equation depicted in Fig. 7.3.

The physical meaning of the Hartree-Fock potential is the interaction between the single particle and the medium (core) made of the remaining $N - 1$ particles. The

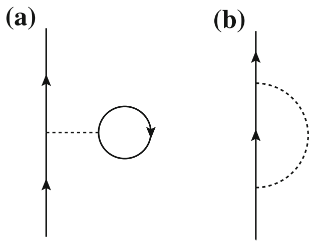

Fig. 7.2 Feynman diagrams representing the Hartree-Fock potential. **a** is the direct contribution (V_{dir}), **b** is the exchange contribution (V_{ex}). Thin lines represent the single particle propagator in the mean-field potential, doted lines represent the inter-particle interaction

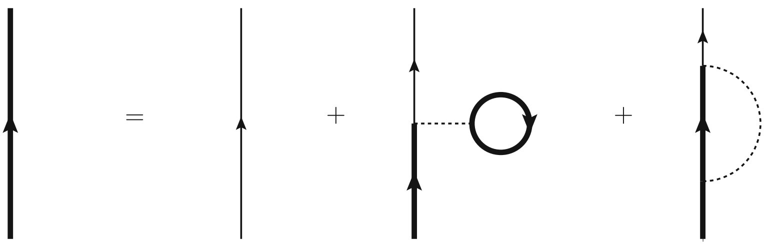

Fig. 7.3 Self-consistent equation for the Hartree-Fock method drawn with Feynman diagrams. Thin lines represent the single particle propagator in the mean-field potential, doted lines represent the interaction. The self-consistent equation will be solved for the thick line

Slater determinant made of Hartree-Fock N particles forms the ground state of the many-body system.

Hartree-Fock method is known to be a very good approximation, but more improvement can be done for the nuclear calculation. In the Hartree-Fock method, the many-body states are Slater determinants formed by the independent single particle states of the mean field. To improve the situation, we should add correlations and introduce the dynamical multi-particle state. We should therefore consider excitations and de-excitations of one-particle states (generated from Hartree-Fock method) through interactions between each other. In this framework, the energy raising operator should be written as

$$X_\eta^\dagger = \sum_{p,h} \left(x_{\eta,ph} a_p^\dagger b_h^\dagger - y_{\eta,ph} b_h a_p \right) \tag{7.43}$$

where a and b are particle and hole annihilating operators, respectively. p and h are the corresponding indices. The determinations of $x_{\eta,ph}$ and $y_{\eta,ph}$ are therefore needed. As $X_\eta^\dagger$'s are energy raising operators, they must satisfy the Heisenberg equation $[H, X_\eta^\dagger] = \hbar\omega_\eta X_\eta^\dagger$. By substituting $X_\eta^\dagger$ and the hamiltonian, we obtain the following equation

$$\begin{aligned}
\hbar\omega_\eta \left(x_{\eta,ph} a_p^\dagger b_h^\dagger - y_{\eta,ph} b_h a_p \right) = & \sum_{p,h} (\epsilon_p - \epsilon_h) x_{\eta,ph} a_p^\dagger b_h^\dagger \\
& + \sum_{p,h,p',h'} (V_{ph'hp'} x_{\eta,p'h'} + V_{pp'hh'} y_{\eta,p'h'} a_p^\dagger b_h^\dagger) \\
& + \sum_{p,h} (\epsilon_p - \epsilon_h) y_{\eta,ph} b_h a_p \\
& + \sum_{p,h,p',h'} (V_{hp'ph'} y_{\eta,p'h'} + V_{hh'pp'} x_{\eta,p'h'} b_h a_p) \\
& + O((a^\dagger b^\dagger, ba)^2)
\end{aligned} \tag{7.44}$$

where V is the particle-hole interaction and higher order terms in $a^\dagger b^\dagger$ and ba are neglected. This self-consistent equation is called the random phase approximation (RPA) equation. The RPA is a dynamical approach: by considering particle-hole interactions, the energy eigenstates of the many-body system become a superposition of particle-hole excitations (see Fig. 7.4).

The Hartree-Fock potential was able to renormalize the interactions between particles into an effective mean-field. The next step is then to include the contribution of the residual interactions. For the nuclear case, the strongest residual interaction is the spin pairing interaction between nucleons. In the presence of attractive pairing interactions, particles can form spin-zero bound-states, which can be effectively seen

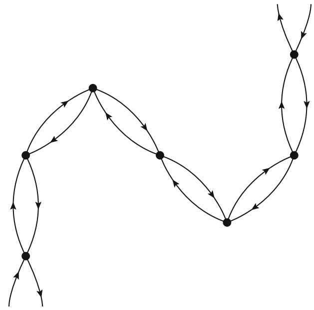

Fig. 7.4 Example of diagrammatic representation of 1-particle 1-hole state in RPA. The black dots are particle-hole interactions. Time axis goes from the bottom to the top. The state is a mixing of states with different number of particle-hole pairs

as *mixing between particles and holes*. The mixing between particles and holes is well described in the BCS theory [22, 23]. The hamiltonian of the nuclear system with pairing force can be written as

$$H = \sum_{\alpha}^{N} \epsilon_a c_\alpha^\dagger c_\alpha - \frac{1}{4} G_0 \left(\sum_{\alpha}^{N} (-1)^{j_a - m_\alpha} c_\alpha^\dagger c_{-\alpha}^\dagger \right) \left(\sum_{\beta}^{N} (-1)^{j_b - m_\beta} c_{-\beta} c_\beta \right) \quad (7.45)$$

where c and $c^\dagger$ are annihilation/creation operator of nucleon. The first term in this equation is the Hartree-Fock diagonalized hamiltonian, and the second term is the pairing force. We can see that this hamiltonian is not diagonal, due to the addition of the pairing. To diagonalize this relation, we need to rotate the basis of particle and hole:

$$\begin{aligned} a_\alpha^\dagger &= u_a c_\alpha^\dagger - v_a \tilde{c}_\alpha \\ \tilde{a}_\alpha &= u_a \tilde{c}_\alpha - v_a c_\alpha^\dagger \end{aligned} \quad (7.46)$$

where $\tilde{c}$ and $\tilde{c}^\dagger$ are the annihilation and creation operators of holes, respectively. $\tilde{a}$ and $\tilde{a}^\dagger$ are the corresponding operators for *quasi-particles*, giving the new basis of physical states. This transformation of basis is the Bogoliubov transformation. The determination of u and v will be done by fitting the energy of the system phenomenologically. The extension of the RPA with this formalism can also be done by considering the quasi-particle excitations. The BCS extension of the RPA is called quasi-particle RPA (QRPA).

Once we have explained the basic formalism for calculating nuclear systems, let us now present the calculation of the nuclear Schiff moments. Early calculation of nuclear moments induced by P, CP-odd nuclear forces was done by Flambaum et al. considering the interaction of the valence nucleon with the core within the phenomenological Woods-Saxon potential as a mean-field [24, 25]. RPA calculations

(Hartree-Fock + non-pairing residual interaction) were done by Dmitriev et al., and the dependence of ^{129}Xe, ^{199}Hg, ^{211}Rn and ^{225}Ra Schiff moments on the P, CP-odd pion-nucleon couplings were given in Ref. [26]. The following P, CP-odd pion-nucleon couplings were included at the first order of perturbation, via the following P, CP-odd nucleon-nucleon interaction:

$$W(\mathbf{r}_a - \mathbf{r}_b) = -\frac{g_{\pi NN}}{8\pi m_p} \Big[\Big(\bar{g}^{(0)}_{\pi NN} \tau_a \cdot \tau_b + \bar{g}^{(2)}_{\pi NN} (\tau_a \cdot \tau_b - 3\tau^z_a \tau^z_b) \Big) (\boldsymbol{\sigma}_a - \boldsymbol{\sigma}_b) + \bar{g}^{(1)}_{\pi NN} (\tau^z_a \boldsymbol{\sigma}_a - \tau^z_b \boldsymbol{\sigma}_b) \Big] \cdot \nabla_a \frac{e^{-m_\pi r_{ab}}}{r_{ab}} \tag{7.47}$$

where a and b denote the indices of the two interacting nucleons, and $r_{ab} \equiv |\mathbf{r}_a - \mathbf{r}_b|$. This P, CP-odd interaction was also used in the *ab initio* evaluation of the deuteron and ^{3}He EDMs [see Eq. (7.2)]. The formula for the nuclear Schiff moment is

$$S = \sum_i \frac{\langle \Psi_0 | \hat{S} | \Psi_i \rangle \langle \Psi_i | W | \Psi_0 \rangle}{E_0 - E_i} + \text{c.c.} \tag{7.48}$$

where $\hat{S}$ is the nuclear Schiff moment operator given in Eq. (7.25), and Ψ_0, Ψ_i are nuclear wave functions unperturbed by P, CP-odd N-N interactions W [see Eq. (7.47)] for ground and excited states, respectively.

The result is

$$S_{\text{Hg}} = g_{\pi NN} \Big(-0.00004 \bar{g}^{(0)}_{\pi NN} - 0.055 \bar{g}^{(1)}_{\pi NN} + 0.009 \bar{g}^{(2)}_{\pi NN} \Big) e\,\text{fm}^3 \tag{7.49}$$

$$S_{\text{Xe}} = g_{\pi NN} \Big(0.008 \bar{g}^{(0)}_{\pi NN} + 0.006 \bar{g}^{(1)}_{\pi NN} - 0.009 \bar{g}^{(2)}_{\pi NN} \Big) e\,\text{fm}^3 \tag{7.50}$$

$$S_{\text{Rn}} = g_{\pi NN} \Big(-0.019 \bar{g}^{(0)}_{\pi NN} + 0.061 \bar{g}^{(1)}_{\pi NN} + 0.053 \bar{g}^{(2)}_{\pi NN} \Big) e\,\text{fm}^3 \tag{7.51}$$

$$S_{\text{Ra}} = g_{\pi NN} \Big(0.033 \bar{g}^{(0)}_{\pi NN} - 0.037 \bar{g}^{(1)}_{\pi NN} - 0.043 \bar{g}^{(2)}_{\pi NN} \Big) e\,\text{fm}^3 \,. \tag{7.52}$$

The small coefficient of $\bar{g}^{(0)}_{\pi NN}$ for the ^{199}Hg Schiff moment is due to an accidental cancellation.

The nucleon EDM dependence of the ^{199}Hg Schiff moment was also calculated in Ref. [27] within the same approach, giving

$$S_{\text{Hg}} = \big((1.895 \pm 0.035) d_n + (0.20 \pm 0.02) d_p \big) \frac{10^{13}}{e\,\text{cm}} e\,\text{fm}^3 \,. \tag{7.53}$$

A more sophisticated calculation including the effects of pairing force with phenomenological Skyrme interactions and nuclear deformation was done for ^{199}Hg [28, 29], ^{211}Rn [29] and for ^{225}Ra [30, 31] Schiff moments. Calculations were made using the computer code HFODD [32] within several models of phenomenological Skyrme interactions: SkO' [33], SkM* [34], SLy4 [35], SV [36] and SIII [36]. SIII

Table 7.1 Coefficients a_i of the dependence of the Schiff moment on P, CP-odd pion-nucleon couplings ($S = g_{\pi NN}(a_0 \bar{g}^{(0)}_{\pi NN} + a_1 \bar{g}^{(1)}_{\pi NN} + a_2 \bar{g}^{(2)}_{\pi NN})$) in unit of e fm^3

Nucleus	Model	$-a_0$	$-a_1$	a_2	$-b$	Ref.
^{199}Hg	SkO'	0.010	0.074	0.018	–	[28]
	SkM* (HFB)	0.041	−0.027	0.069	0.013	
	SLy4 (HFB)	0.013	−0.006	0.024	0.007	[29]
	SLy4 (HF)	0.013	−0.006	0.022	0.003	
	SV (HF)	0.009	−0.0001	0.016	0.002	
	SIII (HF)	0.012	0.005	0.016	0.004	
^{211}Rn	SkM*	0.042	−0.028	0.078	0.015	
	SLy4	0.042	−0.018	0.071	0.016	[29]
	SIII	0.034	−0.0004	0.064	0.015	
^{225}Ra	SkO'	−1.5	6.0	−4.0	–	[31]

The labels HB and HFB stand for calculations in the Hartree-Fock and Hartree-Fock-Bogoliubov approximations, respectively.

may not be as trustworthy as the others: Ref. [28] showed that the interaction was less able to reproduce related observable, the distribution of isoscalar E1 strength in even nuclei. The result is shown in Table 7.1.

The results for ^{211}Rn Schiff moment are almost consistent. The ^{211}Rn nucleus is spherical, so no deformation was considered in the calculations.

In the case of ^{225}Ra Schiff moment, the large enhancement of the P, CP-odd contributions is due to the presence of a nearby parity-doublet states [30]. We have more confidence in the Sko' results, but the uncertainties due to difficulties in treating nuclear deformation in the men-field methods are large. In addition, the optimal Skyrme functional has not yet been identified. These deficiencies render a factor of 2 or 3 of uncertainty [31].

^{199}Hg nucleus has also a small deformation, so it is useful to consider it. The calculation of Ref. [29] took into account the effect of deformation and calculated fully self-consistently, including the P, CP-odd interactions. By comparing with the result of Ref. [28] which considered spherical ^{199}Hg nucleus, we see that the isovector coefficient a_1 significantly decreases with the inclusion of deformation. The results for a_1 vary among Skyrme models and we have no decisive pretext to select one of them.

The calculation of nuclear Schiff moment presents some difficulties in determining the dependence to the P, CP-odd pion-nucleon couplings. This is essentially due to the deficiency in expressing nuclear states of odd nuclei in mean-field theory. To have an accurate description of the nuclei in question, we must wait for new calculational method for odd nuclei. In the subsequent discussion, we will take the average between different calculations shown in Table 7.1 for each coefficient.

7.5 Summary of Nuclear Level Calculation

Deuteron EDM:

$$d_d = -0.015 g_{\pi NN} \bar{g}^{(1)}_{\pi NN} \times 10^{-13} e\,\text{cm} + d_p + d_n \,. \tag{7.54}$$

The deuteron EDM was calculated with realistic N-N potential [6].

^{3}He nucleus EDM:

$$\begin{aligned} d_{\text{He}} =& g_{\pi NN}\left[-0.015\bar{g}^{(0)}_{\pi NN} - 0.023\bar{g}^{(1)}_{\pi NN} + 0.036\bar{g}^{(2)}_{\pi NN}\right] \times 10^{-13} e\,\text{cm} \\ &- 0.04 d_p + 0.90 d_n \end{aligned} \tag{7.55}$$

The ^{3}He nuclear EDM was calculated with the *ab initio* No-core shell model with realistic N-N potential [9].

^{199}Hg nuclear Schiff moment:

$$\begin{aligned} S_{\text{Hg}} =& g_{\pi NN}\Bigg[0.02\bar{g}^{(0)}_{\pi NN} - 0.007\bar{g}^{(1)}_{\pi NN} + 0.006\bar{g}^{(2)}_{\pi NN} \\ &+ \frac{0.91 d_n + 0.09 d_p}{e\,\text{cm}} \times 4 \times 10^{12}\Bigg] e\,\text{fm}^3 \,. \end{aligned} \tag{7.56}$$

This is the average of different calculations of mean-field method presented in Ref. [29].

^{129}Xe nuclear Schiff moment:

$$S_{\text{Xe}} = g_{\pi NN}\left[0.008\bar{g}^{(0)}_{\pi NN} + 0.006\bar{g}^{(1)}_{\pi NN} - 0.009\bar{g}^{(2)}_{\pi NN} - \frac{3.2 d_n + 0.06 d_p}{e\,\text{cm}} \times 10^{12}\right] e\,\text{fm}^3. \tag{7.57}$$

The πNN interaction contribution was given by Dmitriev et al. with mean field method [26]. The nucleon EDM contribution was calculated in the refined shell model by Yoshinaga et al. [37].

^{211}Rn nuclear Schiff moment:

$$S_{\text{Rn}} = g_{\pi NN}\left[-0.039\bar{g}^{(0)}_{\pi NN} + 0.0155\bar{g}^{(1)}_{\pi NN} + 0.071\bar{g}^{(2)}_{\pi NN} + \frac{d_n}{e\,\text{cm}} \times 1.5 \times 10^{13}\right] e\,\text{fm}^3. \tag{7.58}$$

This was calculated with mean field method in Ref. [29].

^{225}Ra nuclear Schiff moment:

$$S_{\mathrm{Ra}} = g_{\pi NN}\left[1.5\bar{g}^{(0)}_{\pi NN} - 6.0\bar{g}^{(1)}_{\pi NN} - 4.0\bar{g}^{(2)}_{\pi NN}\right] e\,\mathrm{fm}^3\,. \tag{7.59}$$

This was calculated with mean field method with octupole deformation taken into account [31].

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