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# TIME DEPENDENT PERTURBATION THEORY AND THE ZEL'DOVICH ELECTRIC DIPOLE MOMENT IN ATOMS

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**Dedicated to Professor Mladen Paić on the occasion of his 90$^{\mathbf{th}}$ birthday**

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We use time dependent perturbation theory to investigate the Zel'dovich electric dipole moment. We show that the vanishing Stark shift and non-vanishing torque arise from different time dependences used in their calculation.

## 1. *Introduction*

As is well known [1,2], the matrix element of the electric dipole moment (EDM) operator $\vec{d} = e\vec{r}$ vanishes in a stable, rotationally invariant system due to parity ($P$) and time reversal ($T$) invariance. However, as suggested by Zel'dovich [3], these arguments need not apply to an unstable system where an arrow of time arises from the exponential decay law. He suggested that a $T$-invariant system, such as an atom in an excited state which is not $P$-invariant (due to the weak interaction), may pos-

sess a non-zero EDM. This "Zel'dovich moment" (ZM) would be proportional to the linewidth $\Gamma$ of the state and to the $P$-violating weak interaction $V^{PV}$. Subsequently, the ZM has been studied by a number of authors [4-13]. Recently, Botz et al. have shown that the Zel'dovich moment may lead to new parity-violating effects in atoms [14].

However, some controversy has surrounded the physical manifestations of the ZM since it does not appear to behave like an ordinary EDM. For example, Bell [4-6] shows that when an atom possessing a ZM is placed in externally applied electric field $\vec{\mathcal{E}}$, there is no linear Stark shift of the energy levels arising from

$$V_A^{dipole} = -\vec{d} \cdot \vec{\mathcal{E}}, \tag{1}$$

and no precession of the excited state angular momentum. This is mysterious since one can show that the torque,

$$\vec{N} = \langle \vec{d} \rangle \times \vec{\mathcal{E}}, \tag{2}$$

need not vanish, and may lead to a torque exerted on a macroscopic system [7]. Bell resolves this apparent contradiction by showing that the missing change in angular momentum appears in the decay products. However, Botz et al. [14] have shown that Bell's argument may not hold in general, and precession may be observed in some excited systems.

In this paper, we hope to shed more light on the unusual behaviour of the ZM. By applying time dependent perturbation theory [15,16], we will see that the absence of a Stark shift, but non-zero torque, arise from the fundamentally different ways these effects are calculated. It will be shown that the end result depends on the boundary conditions which are used in the time dependent formalism. The interaction can either be switched on adiabatically, like

$$e^{-\eta|t|}, \qquad t \to \pm\infty \tag{3}$$

or abruptly, like

$$\theta(t); \qquad 0 \leq t \leq \infty. \tag{4}$$

In the second case, the interaction stays on forever once it is switched on.

We begin in Sec. 2 by establishing a model of an atom interaction with the radiation field. Then in Sec. 3, we use the $S$-matrix formalism to show that the ZM does not give rise to a linear Stark shift if placed in an external electric field, as would be expected. In Sec. 4, we calculate the expectation value of the system's torque $\vec{N}$ which we find to be non-zero. This same argument leads to a non-vanishing EDM in Sec. 5. In Sec. 6 we show another method to obtain a vanishing EDM. We conclude with Sec. 7 where we discuss why these conflicting answers arise.

## *2. System Hamiltonian*

It is convenient to use an atom (hydrogen) to illustrate the effects of the ZM, since it contains all the necessary ingredients (instability and weak interaction), while at the same time being very well understood. Moreover, in recent years substantial experimental effort has been devoted to the search for EDMs in atoms and molecules [17,18]. The instability of atom in an excited state arises from its interaction with the radiation field. Thus, for our system, we use the atom + field system, and write the Hamiltonian $H$ describing the evolution of the total system as

$$H = H_A + H_R + V_{AR}, \tag{5}$$

where $H_A$ represents the total atomic Hamiltonian, $H_R$ is the free Hamiltonian of the radiation field and $V_{AR}$ is the interaction between the atom and field which gives rise to the atomic instability. For example, $V_{AR}$ is the electric dipole interaction to lowest order. For later purposes, we split the atomic Hamiltonian $H_A$ into several parts:

$$H_A = H_A^{(0)} + V_A^{PV} + V_A^{dipole}. \tag{6}$$

Here $H_A^{(0)}$ represents the lowest order $P$-conserving Hamiltonian, i.e.,

$$H_A^{(0)} = \frac{\vec{p}^2}{2m} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}, \tag{7}$$

while $V_A^{PV}$ represents the $P$-violating weak interaction between the nucleus and orbiting electron. We have also included in Eq. (6)

$$V_A^{dipole} = -\vec{d}\cdot\vec{\mathcal{E}}, \tag{8}$$

which is the electric dipole interaction of the atom with an external (classical) electric field $\vec{\mathcal{E}}$. In practice, we can solve the Schrödinger equation for the free Hamiltonian

$$H^{(0)} = H_A^{(0)} + H_R \tag{9}$$

exactly, and treat the remaining interactions $V_A^{PV}$, $V_A^{dipole}$ and $V_{AR}$ perturbatively. That is, we write the total Hamiltonian $H$ as

$$H = H^{(0)} + V, \tag{10}$$

where

$$V = V_{AR} + V_A^{PV} + V_A^{dipole}. \tag{11}$$

The time evolution of the total atom + radiation system is governed by the time evolution operator $U(t,t')$,

$$|\psi(t)\rangle = U(t,t')|\psi(t)\rangle, \tag{12}$$

where $|\psi(t)\rangle$ is the state vector describing the total system at time $t$, and $U(t,t')$ is given by

$$U(t,t') = \mathcal{T}\left(e^{-\mathrm{i}H(t-t')/\hbar}\right). \tag{13}$$

By introducing the resolvent of the total Hamiltonian $H$

$$G = \frac{1}{z-H}, \tag{14}$$

one can show [19] that $U(\tau)$ can be expressed as

$$U(\tau) = \frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{\infty} \mathrm{d}E\, e^{-\mathrm{i}E\tau} \left[G_-(E) - G_+(E)\right], \tag{15}$$

where

$$G_\pm(E) = \lim_{\eta\to 0^+} G(E \pm \mathrm{i}\eta), \tag{16}$$

and $\tau = t - t'$.

While one is unable to determine the exact matrix elements of $G(z)$, one can expand $G(z)$ in powers of the total perturbation $V$ given by Eq. (11) [20],

$$\begin{aligned} G(z) &= G_0(z) + G_0(z)VG(z) \\ &= G_0(z) + G_0(z)VG_0(z) + G_0(z)VG_0(z)VG_0(z) + O(V^3), \end{aligned} \tag{17}$$

where

$$G_0 = \frac{1}{z - H^{(0)}}. \tag{18}$$

The series given in Eq. (17) can be approximately summed in certain cases. For our purposes the most instructive example is the one described in Chapter IIIC of Ref. 16. There one considers the total states of the atom + radiation system, such as

$$\begin{aligned} |\varphi_b\rangle &= |b,0\rangle \\ |\varphi_a\rangle &= |a,\vec{k}\vec{\varepsilon}\rangle. \end{aligned} \tag{19}$$

Here $|a\rangle$ and $|b\rangle$ refer to eigenstates of the unperturbed Hamiltonian of the atom, $H_A^{(0)}$, while $\vec{k}$ and $\vec{\varepsilon}$ describe a photon. In this example, the purely atomic perturbations are neglected, so

$$\tilde{H}^{(0)} = H_A^{(0)} + H_R + V_{AR}, \tag{20}$$

and its corresponding resolvent $\tilde{G}_0$ is defined by

$$\tilde{G}_0 = \frac{1}{z - \tilde{H}^{(0)}}. \tag{21}$$

One can evaluate the diagonal matrix element $\tilde{G}_{0b}(z) = \langle\varphi_b|\tilde{G}_0(z)|\varphi_b\rangle$ using the expansion in Eq. (17). After various approximations [21], one obtains

$$\tilde{G}_{0b}(E \pm \mathrm{i}\eta) = \frac{1}{E - E_b - \hbar\Delta_b \pm \mathrm{i}\hbar\Gamma_b/2}, \tag{22}$$

where $\hbar\Delta_b$ is the energy shift (e.g., Lamb shift) in the excited state, and $\Gamma_b$ is the state's linewidth. In the following, $\Delta_b$ is included in $E_b$ and not shown explicitly.

## 3. *S-matrix and vanishing linear Stark shift*

In this section, we use the $S$-matrix formalism to study any energy shifts arising from the ZM for an atom placed in an external electric field. In the $S$-matrix formalism one encounters the adiabatic time dependence, Eq. (3), and is interested in calculating the overlap [22]

$$\begin{aligned} \langle\psi_f(t \to +\infty)|\psi_i(t \to -\infty)\rangle &= \lim_{\substack{t_2\to+\infty \\ t_1\to-\infty}} \langle U^I(0,t_2)\varphi_f|U^I(0,t_1)\varphi_i\rangle \\ &= \lim_{\substack{t_2\to+\infty \\ t_1\to-\infty}} \langle\varphi_f|U^I(t_2,0)U^I(0,t_1)|\varphi_i\rangle. \end{aligned} \tag{23}$$

Here $U^I(t_2,t_1)$ refers to the time evolution operator in the interaction picture [23], where

$$U^I(t_f,t_i) = e^{\mathrm{i}H^{(0)}t_f/\hbar}U(t_f,t_i)e^{-\mathrm{i}H^{(0)}t_i/\hbar}. \tag{24}$$

$U^I$ in Eq. (23) comprises both the parity violation potential $V_A^{PV}$ and $V_A^{dipole} = -\vec{d}\cdot\vec{\mathcal{E}}$ which depends on the external electric field $\vec{\mathcal{E}}$. One can write [22,24],

$$S_{fi} = \langle\varphi_f|S|\varphi_i\rangle \tag{25}$$

$$= \lim_{T\to\infty}\left[e^{\mathrm{i}E_fT/2\hbar}\langle\varphi_f|U(T/2,-T/2)|\varphi_i\rangle e^{-\mathrm{i}E_iT/2\hbar}\right], \tag{26}$$

where $|\varphi_i\rangle$ and $|\varphi_f\rangle$ are initial and final eigenstates of $H^{(0)}$. Repeating the same steps as in Ref. 16, one ends with the transition matrix

$$\mathcal{T}_{fi}(E) = \langle\varphi_f|V + VG(E+\mathrm{i}\eta)V|\varphi_i\rangle, \tag{27}$$

$$G = G_0 + G_0VG. \tag{28}$$

It is useful to split off the atomic perturbations from the rest of the total Hamiltonian (5):

$$H = \tilde{H}^{(0)} + V_A^{PV} + V_A^{dipole}. \tag{29}$$

Then $G_0$ in Eq. (27) can be assumed to correspond to $\tilde{G}_0$ associated with $\tilde{H}^{(0)}$, Eq. (21), while the potential $V$ is given by

$$V_A = V_A^{PV} + V_A^{dipole}. \tag{30}$$

Then Eq. (27) can be approximated by

$$\begin{aligned} \mathcal{T}_{fi}(E) &\simeq \langle\varphi_f|V_A|\varphi_i\rangle + \langle\varphi_f|V_A\tilde{G}_0(E+\mathrm{i}\eta)V_A|\varphi_i\rangle \\ &\simeq \langle\varphi_f|V_A|\varphi_i\rangle + \sum_j \langle\varphi_f|V_A|\varphi_j\rangle\langle\varphi_j|\tilde{G}_0(E+\mathrm{i}\eta)|\varphi_j\rangle\langle\varphi_j|V_A|\varphi_i\rangle. \end{aligned} \tag{31}$$

Here we have introduced the intermediate states of Eq. (19). The diagonal matrix element $\mathcal{T}_{ii}$ is the level shift arising from $V_A$ acting on the atomic state $|\mathrm{i}\rangle$,

$$\mathcal{T}_{ii}(E) = \sum_j \left(\langle i|V_A^{PV}|j\rangle\langle j|V_A^{dipole}|\mathrm{i}\rangle + \langle i|V_A^{dipole}|j\rangle\langle j|V_A^{PV}|\mathrm{i}\rangle\right) \frac{1}{E_i - E_j + \mathrm{i}\hbar\Gamma_j/2}. \tag{32}$$

Here we have used the fact that diagonal matrix elements of $V_A$ vanish with respect to eigenstates of $H_A^{(0)}$. One can show quite generally that $\mathcal{T}_{ii}$ must vanish if

$$V_A^{PV} \sim \vec{\sigma}\cdot\vec{p} \tag{33}$$

and

$$\vec{d} \sim \vec{r}. \tag{34}$$

It might be instructive to illustrate this in detail for an $s$-wave ground state $|\mathrm{i}\rangle = |g\rangle$ and for an excited $p$-wave state $|e\rangle$, i.e.,

$$\langle\vec{r}|g\rangle = f_s(r)\chi^\nu \tag{35}$$

$$\langle\vec{r}|e\rangle = f_p(r)\vec{\sigma}\cdot\hat{n}\chi^\nu. \tag{36}$$

where $\hat{n} = \vec{r}/r$, $f_s$ and $f_p$ are the radial wave functions, and $\chi^\nu$ are Pauli spinors. One readily calculates

$$\langle g|V_A^{PV}|e\rangle = -\langle e|V_A^{PV}|g\rangle, \tag{37}$$

and

$$\langle g|V_A^{dipole}|e\rangle = \langle e|V_A^{dipole}|g\rangle. \tag{38}$$

Thus, according to Eq. (32), there is no static EDM in atoms:

$$\begin{aligned}\mathcal{T}_{gg}(E) &= \left(\langle g|V_A^{PV}|e\rangle\langle e|V_A^{dipole}|g\rangle + \langle g|V_A^{dipole}|e\rangle\langle e|V_A^{PV}|g\rangle\right)\frac{1}{E_g - E_e + \mathrm{i}\hbar\Gamma_e/2} \\ &= \left(\langle g|V_A^{PV}|e\rangle\langle e|V_A^{dipole}|g\rangle - \langle e|V_A^{dipole}|g\rangle\langle g|V_A^{PV}|e\rangle\right)\frac{1}{E_g - E_e + \mathrm{i}\hbar\Gamma_e/2} \\ &= 0. \end{aligned} \tag{39}$$

Moreover, the interaction with any parity-odd operator $Q$, which satisfies

$$\langle f|Q|\mathrm{i}\rangle = \langle i|Q|f\rangle, \tag{40}$$

also vanishes in atoms.

The physical content of the formalism described above does not correspond to the master equation formalism which was employed in Ref. 25. The formalism of the next section will be based on the same physical assumptions of Chapter 6 in Ref. 25. This connection is illustrated in detail in Sec. 5. Section 6 contains an imperfect attempt to produce an analog of Chapter 8 in Ref. 25.

## 4. *Torque*

As already mentioned in the Introduction, the EDM torque was calculated using Eq. (2) between time-dependent states:

$$\begin{aligned}\vec{N} &= \langle\varphi_a|U^I(0,t)\,(\vec{d}\times\vec{\mathcal{E}})\,U^I(t,0)|\varphi_a\rangle \\ &= \langle\varphi_a|U(0,t)e^{-H_0't/\hbar}e^{H_0't/\hbar}\,(\vec{d}\times\vec{\mathcal{E}})\,U(t,0)e^{-H_0't/\hbar}e^{H_0't/\hbar}U(t,0)|\varphi_a\rangle \\ &= \langle\varphi_a|U(0,t)\,(\vec{d}\times\vec{\mathcal{E}})\,U(t,0)|\varphi_a\rangle. \end{aligned} \tag{41}$$

Here one used the Hamiltonian $\hat{H}^{(0)}$ given by

$$\hat{H}^{(0)} = H^{(0)} - V_A^{dipole}. \tag{42}$$

If $|\varphi_e\rangle$ is some unstable state, i.e., $|\psi(0)\rangle$ in Ref. 7, then the quantity $\vec{N}$ exactly corresponds to the quantity $\langle t|\vec{M}|t\rangle$ in Ref. 7. One must use the representation for $U(\tau)$ given in Ref. 26, according to which

$$\langle\varphi_e|U(0,t) \simeq \langle\varphi_e|\int \mathrm{d}E\,\frac{e^{\mathrm{i}Et/\hbar}}{E - E_e - \mathrm{i}\hbar\Gamma_e/2}\frac{1}{2\pi\mathrm{i}} = \langle\varphi_e|e^{\mathrm{i}(E_e+\mathrm{i}\hbar\Gamma_e/2)t/\hbar}, \tag{43}$$

and

$$U(t,0)|\varphi_e\rangle = e^{-\mathrm{i}(E_e+\mathrm{i}\hbar\Gamma_e/2)t/\hbar}|\varphi_e\rangle. \tag{44}$$

Therefore, we have

$$\vec{N} \simeq \langle\varphi_e| e^{\mathrm{i}(E_e - \mathrm{i}\hbar\Gamma_e/2)t/\hbar} \left(\vec{d}\times\vec{\mathcal{E}}\right) e^{-\mathrm{i}(E_e - \mathrm{i}\hbar\Gamma_e/2)t/\hbar} |\varphi_e\rangle. \tag{45}$$

Here the quantities $E_e$ and $\Gamma_e$ correspond to the Hamiltonian $\hat{H}^{(0)}$ given in Eq. (42). The contributions $V_A^{PV}$ can be included by realizing that $|\varphi_e\rangle$ should not have definite parity. Alternatively, one can expand Eq. (44) as follows:

$$\begin{aligned} U(t,0)|\varphi_e\rangle &= \frac{-1}{2\pi\mathrm{i}} \int \mathrm{d}E e^{-\mathrm{i}Et\hbar} \hat{G}_+(E)|\varphi_e\rangle \\ &= \frac{-1}{2\pi\mathrm{i}} \int \mathrm{d}E e^{-\mathrm{i}Et\hbar} \left(\hat{G}_{0+} + \hat{G}_{0+} V_A^{PV} \hat{G}_{0+} + \cdots\right) |\varphi_e\rangle, \end{aligned} \tag{46}$$

$$\langle\varphi_e|U(0,t) = \frac{1}{2\pi\mathrm{i}} \int \mathrm{d}E e^{\mathrm{i}Et\hbar} \langle\varphi_e| \left(\hat{G}_{0-} + \hat{G}_{0+} V_A^{PV} \hat{G}_{0-} + \cdots\right). \tag{47}$$

Here $\hat{G}_{0\pm}$ refers to the Hamiltonian $\hat{H}^{(0)}$ given in Eq. (42), and can be approximated by Eq. (22) if $|\varphi_e\rangle$ is an excited state.

By introducing a complete set of states $|s\rangle$, one obtains

$$\begin{aligned} \vec{N} &= \frac{-1}{(2\pi\mathrm{i})^2} \int_{-\infty}^{+\infty} \mathrm{d}E\, \mathrm{d}E' e^{\mathrm{i}E't/\hbar} e^{\mathrm{i}Et/\hbar} \\ &\times \Big\{ \sum_s \left[ \langle\varphi_e|\hat{G}_{0-}(E') \left(\vec{d}\times\vec{\mathcal{E}}\right) |s\rangle\langle s|\hat{G}_{0+}(E) V_A^{PV} \hat{G}_{0+}(E)|\varphi_e\rangle \right] \\ &+ \sum_k \left[ \langle\varphi_e|\hat{G}_{0-}(E') V_A^{PV} \hat{G}_{0-}|k\rangle\langle k| \left(\vec{d}\times\vec{\mathcal{E}}\right) \hat{G}_{0+}(E)|\varphi_e\rangle \right] \Big\}. \end{aligned} \tag{48}$$

Using

$$\hat{G}_{0\pm}(E)|\varphi_n\rangle = \frac{1}{E - E_n \pm \mathrm{i}\hbar\Gamma_n/2} |\varphi_n\rangle, \tag{49}$$

one finds

$$\vec{N} = \frac{-1}{(2\pi\mathrm{i})^2} \int_{-\infty}^{+\infty} \mathrm{d}E\, \mathrm{d}E' e^{\mathrm{i}E't/\hbar} e^{\mathrm{i}Et/\hbar} \Big\{ \sum_s \Big[$$

$$\langle\varphi_e| \frac{\vec{d}\times\vec{\mathcal{E}}}{E' - E_e - \mathrm{i}\hbar\Gamma_e/2} |s\rangle\langle s| \frac{1}{E - E_s + \mathrm{i}\hbar\Gamma_s/2} V_A^{PV} \frac{1}{E - E_e + \mathrm{i}\hbar\Gamma_e/2} |\varphi_e\rangle \tag{50}$$

$$+ \langle\varphi_e| \frac{1}{E' - E_e - \mathrm{i}\hbar\Gamma_e/2} V_A^{PV} \frac{1}{E' - E_s - \mathrm{i}\hbar\Gamma_s/2} |s\rangle\langle s| \frac{\vec{d}\times\vec{\mathcal{E}}}{E - E_e + \mathrm{i}\hbar\Gamma_e/2} |\varphi_e\rangle \Big] \Big\}.$$

The expression in Eq. (50) can be easily integrated. It contains both $\hat{G}_+$ and $\hat{G}_-$, so it will not vanish. Observe that Eq. (32) has similar character, but contains only $G_+$ and hence vanishes. It seems that only expressions which contain $G_+$ and $G_-$ can "beat" the $T$-invariance cancellation.

## 5. *Non-vanishing EDM*

Since $\vec{N} = \vec{d} \times \vec{\mathcal{E}}$ where $\vec{\mathcal{E}}$ is a $c$-number, the final result Eq. (50) also holds for the expectation value of the EDM operator $\vec{d}$. Thus, one can obtain $\langle \vec{d} \rangle$ by simply replacing $\vec{d} \times \vec{\mathcal{E}}$ with $\vec{d}$ in Eq. (50). If one looks for the ground state EDM, one should specify $|\varphi_e\rangle$ to be an $s$-wave ground state $|g\rangle$, while $|\varphi_s\rangle$ corresponds to an excited $p$-wave state $|e\rangle$, as in Eq. (32). As the ground state has no decay width, one should make the following substitutions in Eq. (50):

$$\mathrm{i}\hbar\Gamma_e/2 \;\rightarrow\; \eta, \tag{51}$$

$$E_e \;\rightarrow\; E_g, \tag{52}$$

$$E_s \;\rightarrow\; E_e, \tag{53}$$

$$\Gamma_s \;\rightarrow\; \Gamma_e. \tag{54}$$

Here the state $|g\rangle$ is the ground state with no photons present:

$$|g\rangle = |\varphi_g\rangle = |g;0\rangle. \tag{55}$$

This leads to the expression

$$\vec{\mathcal{D}}_{gg} = \frac{1}{4\pi^2} \int_{-\infty}^{+\infty} \mathrm{d}E\, \mathrm{d}E' e^{\mathrm{i}E't/\hbar} e^{\mathrm{i}Et/\hbar}$$

$$\langle g| \left\{ \sum_b \Big[ \frac{\vec{d}}{E' - E_g - \mathrm{i}\eta} |b\rangle\langle b| \frac{1}{E - E_b + \mathrm{i}\hbar\Gamma_b/2} V_A^{PV} \frac{1}{E - E_g + \mathrm{i}\eta} |g\rangle \right.$$

$$\left. + \langle g| \frac{1}{E' - E_g - \mathrm{i}\eta} V_A^{PV} \frac{1}{E' - E_b - \mathrm{i}\hbar\Gamma_b/2} |b\rangle\langle b| \frac{\vec{d}}{E - E_g + \mathrm{i}\eta} |g\rangle \Big] \right\}. \tag{56}$$

Obviously, a physical EDM should correspond to the limit $t \to \infty$, i.e., one has to determine $\vec{\mathcal{D}}_{gg}(\infty)$. This limit is also analogous to the steady-state solution in Ref. 25. One can use contour integration to evaluate Eq. (56). Let

$$I_1(t) \;=\; \int_{-\infty}^{+\infty} \mathrm{d}E\, \mathrm{d}E' e^{\mathrm{i}E't/\hbar} e^{-\mathrm{i}Et/\hbar} \frac{1}{(E' - E_g - \mathrm{i}\eta)(E - E_b + \mathrm{i}\hbar\Gamma_b/2)(E - E_g + \mathrm{i}\eta)}$$

$$= 4\pi^2 e^{\mathrm{i}E_g t/\hbar}\left[\frac{e^{-\mathrm{i}E_g t/\hbar}}{E_g - E_b + \mathrm{i}\hbar\Gamma_b/2} + \frac{e^{-i(E_b - \mathrm{i}\hbar\Gamma_b/2)t/\hbar}}{E_b - E_g - \mathrm{i}\hbar\Gamma_b/2}\right], \tag{57}$$

and

$$I_2(t) = \int_{-\infty}^{+\infty} \mathrm{d}E\,\mathrm{d}E' e^{\mathrm{i}E't/\hbar} e^{-\mathrm{i}Et/\hbar} \frac{1}{(E' - E_g - \mathrm{i}\eta)(E' - E_b - \mathrm{i}\hbar\Gamma_b/2)(E' - E_g + \mathrm{i}\eta)}$$

$$= 4\pi^2 e^{-\mathrm{i}E_g t/\hbar}\left[\frac{e^{\mathrm{i}E_g t/\hbar}}{E_g - E_b - \mathrm{i}\hbar\Gamma_b/2} + \frac{e^{i(E_b + \mathrm{i}\hbar\Gamma_b/2)t/\hbar}}{E_b - E_g + \mathrm{i}\hbar\Gamma_b/2}\right], \tag{58}$$

where

$$I_1(\infty) = I_2^*(\infty) = 4\pi^2 \frac{1}{E_g - E_b + \mathrm{i}\hbar\Gamma_b/2}. \tag{59}$$

Thus,

$$\vec{\mathcal{D}}_{gg}(\infty) = \sum_b \left[\frac{\langle g|V_A^{PV}|b\rangle\langle b|\vec{d}|g\rangle}{E_g - E_b - \mathrm{i}\hbar\Gamma_b/2} + \frac{\langle g|\vec{d}|b\rangle\langle b|V_A^{PV}|g\rangle}{E_g - E_b + \mathrm{i}\hbar\Gamma_b/2}\right]. \tag{60}$$

This result should be compared with $\mathcal{T}_{gg}$ given in Eq. (39). The product $\vec{\mathcal{E}}\cdot\vec{\mathcal{D}}_{gg}(\infty)$ has the same dimension as in Eq. (39). The only difference is in the energy denominators. If Eq. (39) vanishes, as discussed in Sec. 3, then Eq. (60) does not. The non-zero contribution is proportional to $\Gamma_b$, and is analogous to Eq. (7.34) of Ref. 25.

## 6. *Vanishing EDM*

If some approximations are assumed, a conclusion analogous to the result found in Chapter 8 of Ref. [25] can be obtained in a trivial way. Instead of the Hamiltonian given in Eqs. (5) and (11), one should use Eq. (42)

$$H = \hat{H}^{(0)} + V_{AR}, \tag{61}$$

where

$$\hat{H}^{(0)} = H^{(0)} + V_A^{PV}. \tag{62}$$

Here $\hat{H}^{(0)}$ plays the role of $H^{(0)}$ in Eq. (9). The states of the atom + radiation system are now,

$$\begin{aligned} |\hat{\varphi}_b\rangle &= |\hat{b}, 0\rangle \\ |\hat{\varphi}_g\rangle &= |\hat{g}, \vec{k}\vec{\varepsilon}\rangle. \end{aligned} \tag{63}$$

Neither $|\hat{b}\rangle$ nor $|\hat{g}\rangle$ conserves parity. They are eigenstates of the Hamiltonian $\hat{H}^{(0)}$, and can be approximated by

$$|\hat{g}\rangle = |g\rangle - \sum_b |b\rangle \frac{\langle b|V_A^{PV}|g\rangle}{E_b - E_g} + O(V_A^{PV})^2. \tag{64}$$

Using Eqs. (4) and (5), one can write

$$\vec{\mathcal{D}}_{\hat{g}\hat{g}} = \frac{1}{4\pi^2} \int_{-\infty}^{+\infty} \mathrm{d}E\, \mathrm{d}E' e^{\mathrm{i}E't/\hbar} e^{-\mathrm{i}Et/\hbar} \langle \hat{g}|\hat{G}_-(E')\vec{d}\hat{G}_+(E)|\hat{g}\rangle, \tag{65}$$

where

$$\hat{G}(z) \equiv \langle \hat{g}|G|\hat{g}\rangle = \frac{1}{z - \hat{E}_g}. \tag{66}$$

Here $\hat{E}_n$ are eigenvalues of $\hat{H}^{(0)}$. If one introduces the intermediate states in Eq. (65), and approximates the sum with just a ground state, i.e.,

$$\sum_l |\varphi_l\rangle\langle\varphi_l| \simeq |\hat{g}\rangle\langle\hat{g}|, \tag{67}$$

one obtains

$$\begin{aligned} \vec{\mathcal{D}}_{\hat{g}\hat{g}} &\simeq \frac{1}{4\pi^2} \int_{-\infty}^{+\infty} \mathrm{d}E\, \mathrm{d}E' e^{\mathrm{i}E't/\hbar} e^{-\mathrm{i}Et/\hbar} \frac{1}{E' - \hat{E}_g - \mathrm{i}\eta} \frac{1}{E - \hat{E}_g + \mathrm{i}\eta} \langle \hat{g}|\vec{d}|\hat{g}\rangle \\ &= \langle \hat{g}|\vec{d}|\hat{g}\rangle. \end{aligned} \tag{68}$$

When the state $|\hat{g}\rangle$ is approximated by Eq. (64), one obtains an expression which is analogous to Eq. (32), which also vanishes. The difference between the nonvanishing $\vec{\mathcal{D}}_{gg}(\infty)$ and the vanishing of $\vec{\mathcal{D}}_{\hat{g}\hat{g}}(\infty)$ arises from the different definition of the "physical" ground state. In the first case, the ground state is supposed to be an eigenvector of Hamiltonian $\hat{H}^{(0)}$ given in Eq. (42), which is given approximately by

$$|g_{PV}\rangle = |g\rangle - \sum_b |b\rangle \frac{\langle b|V_A^{PV}|g\rangle}{E_b - E_g + \mathrm{i}\hbar\Gamma_b/2}. \tag{69}$$

Here $|g\rangle$ and $|b\rangle$ are eigenvectors of the Hamiltonian $H^{(0)}$. In the second case, the "physical" ground state is the eigenvector of the Hamiltonian $\hat{H}^{(0)}$, Eq. (42), and its approximate expression is given by Eq. (64). Thus, Eq. (68) is to be compared with

$$\vec{\mathcal{D}}_{gg}(\infty) = \langle g_{PV}|\vec{d}|g_{PV}\rangle. \tag{70}$$

While the "physical" ground state Eq. (64) is defined with the electromagnetic $V_{AR}$ interaction being absent, the choice in Eq. (69) contains, at least to some extent, the electromagnetic corrections. It seems that one might fairly argue that the state $|g_{PV}\rangle$ might be closer to the physical reality than $|\hat{g}\rangle$.

Some additional, but inessential complications in the evaluation of $\vec{\mathcal{D}}_{gg}$ appear if the set of intermediate states Eq. (67) is enlarged to

$$\sum_l |\varphi_l\rangle\langle\varphi_l| \simeq |\hat{g}\rangle\langle\hat{g}| + |\hat{b};\vec{k},\vec{\epsilon}\rangle\langle\hat{b};\vec{k},\vec{\epsilon}|. \tag{71}$$

Then one encounters contributions of the form

$$\begin{aligned}\vec{\mathcal{D}}_{\hat{g}\hat{g}}(2nd) &= \frac{1}{4\pi^2}\int_{-\infty}^{+\infty} \mathrm{d}E\,\mathrm{d}E' e^{\mathrm{i}E't/\hbar} e^{-\mathrm{i}Et/\hbar} \\ &\quad \times \sum_{\vec{k},\vec{\varepsilon}} \langle\hat{g}|G_-(E')|\hat{b}\rangle\langle\hat{b}|\vec{d}|\hat{b}\rangle\langle\hat{b}|G_+(E)|\hat{g}\rangle. \end{aligned}\tag{72}$$

As $\langle\hat{b}|\vec{d}|\hat{g}\rangle$ must vanish, this is the only possible additional contribution. However, using

$$|\hat{b}\rangle \simeq |b\rangle - |\mathrm{i}\rangle\frac{\langle g|V_A^{PV}|b\rangle}{E_g - E_b}, \tag{73}$$

$$\langle\hat{b}|\vec{d}|\hat{b}\rangle = 0. \tag{74}$$

## 7. *Conclusion*

When one describes the influences of external fields (in this case of a static electric field $\vec{\mathcal{E}}$), the "time character" of the interaction is of particular importance. One can have an adiabatic switching–on (AS) of the interaction, with time dependence $e^{-\eta|t|}$. In that case, which corresponds to the formalism in Sec. 3, there is no interaction when $t \to \pm\infty$. This should be compared with the abrupt switching–on (AA) of the interaction ($\theta(t)$ time dependence) as used in Sec. 4. Obviously, if the influence of $Q$ was calculated using AA, one would have obtained a nonvanishing result. With AS, there would be no torque. In the language of Ref. 27, one should use in our Sec. 3 the left $\langle\overline{m}|$ and the right $|n\rangle$ eigenvectors. The results of Sec. 4 can be obtained by using the right eigenvectors only. The vanishing EDM result obtained in Ref. 25 is to some extent mimicked in Sec. VI. When the electroweak interactions $V_{AR}$ and $V_A^{PV}$ are included, the results depend on the correct identification of the "physical" atomic state.

Thus, the theoretical conclusions depend crucially on the decision as to which formal aspect of the theory, i.e., AA or AS ($|g_{PV}\rangle$ or $|\hat{g}\rangle$) correctly describes the

physical world which is investigated by a particular experiment. A theoretical formalism might be mathematically perfectly consistent, and yet inadequately describe the real world if the wrong boundary conditions (e.g., AS rather than AA) or improper state vectors are chosen.

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## VREMENSKI OVISNA PERTURBACIJSKA TEORIJA I ZELDOVIČEV ELEKTRIČNI DIPOL U ATOMIMA

Vremenski ovisna perturbacijska teorija upotrebljena je za izučavanje Zeldovičevog električnog dipolnog momenta. Pokazano je da iščezavajući Starkov pomak i neiščezavajuća torzija nastaju zbog različite vremenske ovisnosti primijenjene u računima.