EDM Hamiltonian

Consider a system with two levels of opposite parity (A and B), which have the same J and M and are separated in energy by Δ. In the presence of an electric field along the z-axis, the Hamiltonian is:

$$\mathbf{H1} = \begin{pmatrix} 0 & dE \\ dE & \Delta \end{pmatrix}$$

We can find the eigenvalues for this system:

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Solve[-λ (Δ - λ) - (dE)^2 == 0, λ]
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$$\left\{\left\{\lambda \to \frac{1}{2}\left(\Delta - \sqrt{4\,dE^2 + \Delta^2}\right)\right\}, \left\{\lambda \to \frac{1}{2}\left(\Delta + \sqrt{4\,dE^2 + \Delta^2}\right)\right\}\right\}$$

Of course, we have just reproduced the familiar quadratic Stark effect. Note that when |dE|>>|Δ|, we can neglect Δ, and the Stark shifts are linear in dE. Naturally, this has nothing to do with T-violation that forbids linear Stark shifts for non-degenerate systems. (There are handbooks that list "permanent electric dipole moments" of molecules. In fact these are not so, but the condition |dE|>>|Δ| is satisfied for these molecules at very low electric fields because of the small intervals between states of opposite parity.)

Let us now see how the presence of various interactions changes the Hamiltonian. Let us start with P-odd,T-even weak interaction. This interaction mixes levels of opposite parity, thus the non-zero matrix element corresponding to it should appear off the diagonal. For reasons that will become clear very shortly, the matrix element should be pure imaginary, therefore, we have:

$$\mathbf{H2} = \begin{pmatrix} 0 & dE + i\,\delta \\ dE - i\,\delta & \Delta \end{pmatrix}$$

We write $-i\,\delta$ in the lower left element, so the resulting matrix is Hermitian (so the eigenvalues, i.e. energies, come out real):

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Solve[-λ (Δ - λ) - (dE + i δ) (dE - i δ) == 0, λ]
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$$\left\{\left\{\lambda \to \frac{1}{2}\left(\Delta - \sqrt{4\,dE^2 + 4\,\delta^2 + \Delta^2}\right)\right\}, \left\{\lambda \to \frac{1}{2}\left(\Delta + \sqrt{4\,dE^2 + 4\,\delta^2 + \Delta^2}\right)\right\}\right\}$$

We see that the P-odd,T-even interaction, although it mixes the two oppsite parity states, does not lead to linear (i.e. first-order in dE) Stark shifts. For completeness, let us also add terms that describe decay of the states A and B. Note that in this case, the resulting effective Hamiltonian is non-Hermitian.

$$\mathbf{H3} = \begin{pmatrix} -i\,\Gamma a/2 & dE + i\,\delta \\ dE - i\,\delta & \Delta - i\,\Gamma b/2 \end{pmatrix}$$

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Solve[(-i Γa / 2 - λ) (Δ - i Γb / 2 - λ) - (dE + i δ) (dE - i δ) == 0, λ]
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$$\left\{\left\{\lambda \to \frac{1}{4}\left(-i\,\Gamma a - i\,\Gamma b + 2\,\Delta - \sqrt{16\,dE^2 - \Gamma a^2 + 2\,\Gamma a\,\Gamma b - \Gamma b^2 + 16\,\delta^2 + 4\,i\,\Gamma a\,\Delta - 4\,i\,\Gamma b\,\Delta + 4\,\Delta^2}\right)\right\},\right.$$
$$\left.\left\{\lambda \to \frac{1}{4}\left(-i\,\Gamma a - i\,\Gamma b + 2\,\Delta + \sqrt{16\,dE^2 - \Gamma a^2 + 2\,\Gamma a\,\Gamma b - \Gamma b^2 + 16\,\delta^2 + 4\,i\,\Gamma a\,\Delta - 4\,i\,\Gamma b\,\Delta + 4\,\Delta^2}\right)\right\}\right\}$$

Once again, there are no linear Stark shifts. Finally, the way to introduce the P-odd,T-odd interaction leading to a permanent electric dipole moment (EDM) is:

$$\mathbf{H4} = \begin{pmatrix} 0 & dE + \epsilon \\ dE + \epsilon & \Delta \end{pmatrix}$$

Solve$[-\lambda\,(\Delta - \lambda) - (dE + \epsilon)^2 == 0,\ \lambda]$

$$\left\{\left\{\lambda \to \frac{1}{2}\left(\Delta - \sqrt{4\,dE^2 + \Delta^2 + 8\,dE\,\epsilon + 4\,\epsilon^2}\right)\right\},\ \left\{\lambda \to \frac{1}{2}\left(\Delta + \sqrt{4\,dE^2 + \Delta^2 + 8\,dE\,\epsilon + 4\,\epsilon^2}\right)\right\}\right\}$$

These eigenvalues correspond to linear Stark shifts. Indded,

Series$\left[\sqrt{4\,dE^2 + \Delta^2 + 8\,dE\,\epsilon + 4\,\epsilon^2},\ \{\epsilon, 0, 1\}\right]$

$$\sqrt{4\,dE^2 + \Delta^2} + \frac{4\,dE\,\epsilon}{\sqrt{4\,dE^2 + \Delta^2}} + O[\epsilon]^2$$

Now it is clear why we wrote the P-odd,T-even weak interaction matrix element as pure imaginary. This is exactly to avoid the appearance of an EDM and T-violation.