J Math Chem (2015) 53:1649–1650
DOI 10.1007/s10910-015-0518-2

LETTER TO THE EDITOR

About the crossing of the energy levels of a parameter-dependent quantum-mechanical Hamiltonian

Francisco M. Fernández[1]

Received: 11 May 2015 / Accepted: 15 May 2015 / Published online: 21 May 2015

Abstract The purpose of this letter is to correct the lack of generality of one of the statements put forward in a recent article about the noncrossing rule in quantum mechanics. We illustrate the point by means of an exactly solvable model.

Keywords Avoided crossings · Noncrossing rule · Parameter-dependent operators

In a recent paper [1] we analyzed the avoided crossings between pairs of eigenvalues of parameter-dependent Hamiltonian operators and considered the well known fact that eigenvalues of the same symmetry do not cross. Typically two such eigenvalues $E_m(\lambda)$ and $E_n(\lambda)$ approach each other when $\lambda < \lambda_0$ and move apart when $\lambda > \lambda_0$ in such way that they appear to repel each other. We argued that under such conditions there is either $\lambda = \lambda_m$ such that $E'_m(\lambda_m) = 0$ or there is $\lambda = \lambda_n$ such that $E'_n(\lambda_n) = 0$ or both. Here we want to point out that this statement may only be valid when the slopes $E'_m(\lambda)$ and $E'_n(\lambda)$ have opposite signs for $\lambda < \lambda_0$. In general, we speak of an avoided crossing when $[E_m(\lambda) - E_n(\lambda)]^2$ exhibits a minimum nonzero value at some point $\lambda = \lambda_0$. The correct condition should therefore be

$$E'_m(\lambda_0) = E'_n(\lambda_0). \tag{1}$$

As a trivial illustrative example, consider the Hamiltonian matrix

$$\mathbf{H} = \begin{pmatrix} 1+\lambda & 0.1 \\ 0.1 & -1+3\lambda \end{pmatrix}. \tag{2}$$

✉ Francisco M. Fernández
fernande@quimica.unlp.edu.ar

1 División Química Teórica, INIFTA (UNLP, CCT La Plata-CONICET), Blvd. 113 S/N, Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina

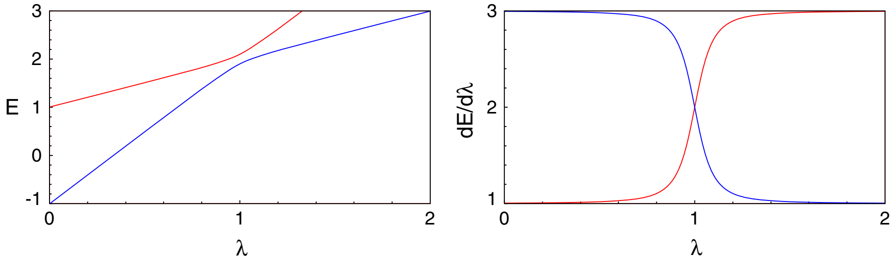

Fig. 1 Eigenvalues $E(\lambda)$ of the Hamiltonian matrix (2) (*left panel*) and their derivatives (*right panel*)

Its eigenvalues exhibit an avoided crossing at $\lambda_0 = 1$ as shown in Fig. 1 and their slopes never vanish. The right panel clearly shows that the slopes are always positive and become equal at $\lambda = 1$ in agreement with Eq. (1).

A nontrivial example with most interesting avoided crossings that illustrate what has just been said was recently discussed elsewhere [2].

References

1. F.M. Fernández, J. Math. Chem. **52**, 2322 (2014)
2. P. Amore, F.M. Fernández, On the symmetry of three identical interacting particles in a one-dimensional box. arXiv:1504.01762 [math-ph]