On the Nonconservation of the Number of Nodal Cells of Eigenfunctions.

M. CAFFAREL, X. KROKIDIS and C. MIJOULE

Laboratoire Dynamique des Interactions Moléculaires, Université Paris VI
75252 Paris Cedex 05, France

Abstract. – The theorem stating that the number of nodal cells of a pure eigenfunction of a Hamiltonian with a smooth and uniformly bounded potential may change as the potential is continuously varied, is illustrated by constructing a particular two-dimensional Hamiltonian (two coupled oscillators) of which one of the eigenfunctions exhibits the nonconservation property. The analytical form of both the potential (a six-order polynomial) and the eigenfunction is given.

Very little is known about the properties of the nodes of eigenfunctions of multidimensional systems. Paraphrasing Korsch[1] we may summarize the few established properties as follows (here n labels the nondegenerate eigenvalues, E_n, $n = 1, 2, 3, ...$, ordered according to increasing magnitude; for simplicity, the properties are expressed for a two-dimensional case):

1) The only state having no nodes is the ground state, $n = 1$.

2) The number of nodal cells of the n-th eigenfunction is not larger than n[2].

3) The number of nodal cells does not necessarily increase with n.

4) The nodal set is generically a manifold; in particular it means that in most cases nodal lines do not cross in the interior of the domain of the Hamiltonian; however, crossings of nodal lines are expected at the boundary[3, 4].

5) If q nodal lines cross, the crossing occurs at equal angles π/q, in particular at right angles for $q = 2$[5].

6) The total length of the nodal lines in state n is bounded from below and increases with n faster than $n^{1/2}$[6].

7) For a Hamiltonian with a uniformly bounded potential and a given energy the volumes of the nodal cells are bounded from below[7] (strictly greater than zero).

An additional property which has been discussed is whether or not the number of nodal cells of a given eigenfunction is conserved when a parameter of the Hamiltonian is continuously varied. A proof that this number is conserved (adiabatic invariant) has been

given by Robnik [7], but was very soon later on criticized by him as containing a gap [8] (events such as the merging of two nodal cells along an $(N - 2), (N - 3), ...,$ 0-dimensional boundary in an N-dimensional configuration space were not considered, and indeed we shall construct below our counterexample in that way). Numerical calculations performed by Korsch [1] for a rectangular «billiard» deformed into a parallelogram demonstrated that the number of nodal cells can change when deforming boundary conditions. A similar conclusion may be drawn from a number of numerical calculations done to study the connection between nodal patterns of nodal lines of eigenfunctions in the semi-classical regime and «quantum chaos» (see, *e.g.*, [9-11]). However, it is generally considered that the number of nodal cells in almost all cases is a conserved quantity, particularly when the energy spectrum is nondegenerate [8]. To our knowledge, no exact eigenfunction of a nontrivial system changing its number of nodal cells under a smooth variation of the potential has been exhibited so far.

The motivation of the present work takes its origin in a recent proposal [12] of computing the fundamental excitations of coupled oscillators with quantum Monte Carlo (QMC). In this scheme—relying essentially on a generalization of the fixed-node approach for excited states—a basic assumption on the nodal structure of eigenfunctions associated with fundamental excitations was made. More precisely it was assumed that their nodes divide the N-dimensional space (N oscillators) into exactly *two* domains. Such an assumption was considered as reasonable since, by their very definition, the fundamental excitations are connected continuously (when decreasing the coupled part of the potential) to the fundamental excitations of some N uncoupled oscillators which, indeed, have this property. However, although numerical calculations for some model and realistically coupled anharmonic oscillators (compared to the exact results obtained by diagonalizing H using a large enough Hermite-Gaussian basis set) have strongly supported our basic assumption, an eventual breakdown of the conservation property could occur. Let us now construct such a situation for a system of two coupled oscillators.

We consider the following wave function:

$$\psi(x, y, \lambda) = f(x, y, \lambda) \exp\left[- \Phi(x, y, \lambda)\right], \tag{1}$$

where Φ is a smooth and bounded function, f some function determining the nodes of ψ via the relation $f = 0$, and λ a parameter controlling the deformation of the nodal pattern. The function Φ is chosen so that ψ describes a bound state, that is $\Phi \to + \infty$ when $|x|$ or $|y|$ tend to infinity (a polynomial form for f being used here, the large-distance behaviour of ψ is determined by Φ). Let us choose f as the simplest function exhibiting the nonconservation property when varying λ. We take

$$f = y^2 - x^3 - F(\lambda)\, x - \frac{2}{27}\,, \tag{2}$$

where $F(\lambda)$ is some function of λ. Regarding the nodal structure of f (or ψ) three different regimes have to be distinguished:

   i) When $F(\lambda) > - 1/3$ the nodes of f divide the plane into two regions.

   ii) At the critical value $F(\lambda) = - 1/3$ the nodal line crosses itself at the singular point $\Omega(1/3, 0)$. Note that f has been chosen so that the crossing is at right angles as required by the property 5) stated above.

   iii) For $F(\lambda) < - 1/3$ the nodes divide the plane into three nodal cells.

The three different regimes are represented in fig. 1. It should be pointed out that condition (7) forbids the emergence of an extra nodal cell from an isolated point of the plane

(the volume of a nodal cell cannot be arbitrarily small at a given energy). Deforming a nodal line in the way just described above circumvents this problem. The next step consists in showing that the wave function (1) may be interpreted as an eigenfunction of a physical Hamiltonian H, namely

$$H\psi = E\psi, \tag{3}$$

where

$$H = -\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x, y, \lambda) \tag{4}$$

and V is a bounded potential function to be determined. Using eqs. (1), (3) and (4) V may be written as follows:

$$V = E + \frac{1}{2}\{(\nabla\Phi)^2 - \nabla^2\Phi\} + \frac{1}{2}\frac{\nabla^2 f}{f} - \frac{\nabla f}{f}\cdot\nabla\Phi. \tag{5}$$

The first three terms of the r.h.s. of (5) are bounded at any finite distances and therefore do not introduce any difficulty (the imposition of the adequate large-distance behaviour of V and ψ will be treated later). In contrast, dividing by f in the last two terms may lead to unphysical divergencies in the potential at the nodes. Therefore, we shall seek a solution for Φ verifying

$$\frac{1}{2}\frac{\nabla^2 f}{f} - \frac{\nabla f}{f}\cdot\nabla\Phi = K(x, y), \tag{6}$$

where K is any bounded function well behaved at large distances. Equation (6) may be rewritten under the form

$$\frac{\partial\Phi}{\partial x}Q(x) + \frac{\partial\Phi}{\partial y}R(y) = S(x, y) \tag{7}$$

with

$$Q(x) = -3x^2 - F, \qquad R(y) = 2y, \qquad S(x, y) = -Kf + 1 - 3x.$$

It turns out that there exists a polynomial solution of eq. (7) when K is also chosen to be polynomial. The simplest (lowest-order) form for K is

$$K(x, y) = K_0 + K_1 x + K_2 x^2 + K_3 y^2, \tag{8}$$

the solution Φ having the form

$$\Phi(x, y) = \sum_{i+j\leqslant 4} a_{ij} x^i y^j. \tag{9}$$

The only nonzero coefficients a_{ij} are

$$a_{10} = -\frac{1}{F}\left(1 + \frac{2K_0}{27}\right), \tag{10a}$$

$$a_{20} = -\frac{1}{2F}\left(K_0 F + \frac{2K_1}{27} - 3\right), \tag{10b}$$

$$a_{30} = -\frac{K_1}{9}, \tag{10c}$$

$$a_{40} = -\frac{K_2}{12}, \tag{10d}$$

$$a_{02} = -\frac{K_0}{4} - \frac{FK_1}{16} + \frac{(4 + 9F^2)}{216}K_3, \tag{10e}$$

$$a_{12} = -\frac{K_1}{4} + \frac{K_3 F}{6}, \tag{10f}$$

$$a_{22} = -\frac{K_3}{6}, \tag{10g}$$

$$a_{04} = -\frac{K_3}{8}. \tag{10h}$$

In addition, the coefficients K_0, K_1, and K_3 are related via the following equalities:

$$K_0 = \frac{F}{3}K_2 + \frac{27}{2}\left(\frac{F^2}{P} - 1\right), \tag{11a}$$

$$K_1 = \frac{9}{2P}, \tag{11b}$$

$$K_2 = \frac{K_3}{2}\left(1 + \frac{1 + 27F^3}{27P}\right) - \frac{27}{8P}, \tag{11c}$$

where

$$P \equiv F^2 - \frac{F}{3} + \frac{1}{9} \tag{11d}$$

is a strictly positive function of λ. In order to get an eigenfunction describing a bound state, the higher-order coefficients a_{40}, a_{04}, and a_{22} determining the large-distance behaviour of ψ and V must all be strictly positive. From eqs. (10) it follows that coefficients K_2 and K_3 must be strictly negative. Finally, since no particular conditions hold for K_0 and K_1, any choice of strictly negative coefficients K_2 and K_3 verifying eq. (11c) is a solution of our problem. We shall exemplify this by choosing K_3 so that coefficient a_{12} (eq. (10f)) vanishes, i.e. $K_3 = 3K_1/2F$. From eqs. (11b), (11c), and (11d) it is easy to check that this is a valid choice if F is taken to be negative. Note that the only requirement on F to obtain a wave function
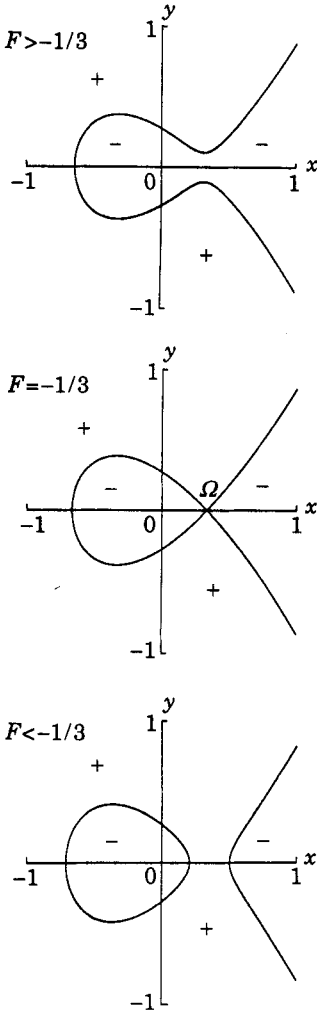
Fig. 1.

Fig. 2.

Fig. 1. – Nodal pattern of the wave function ψ, eq. (1). The three different regimes depending on parameter F are shown. Ω is the singular point where the two nodal cells separate.

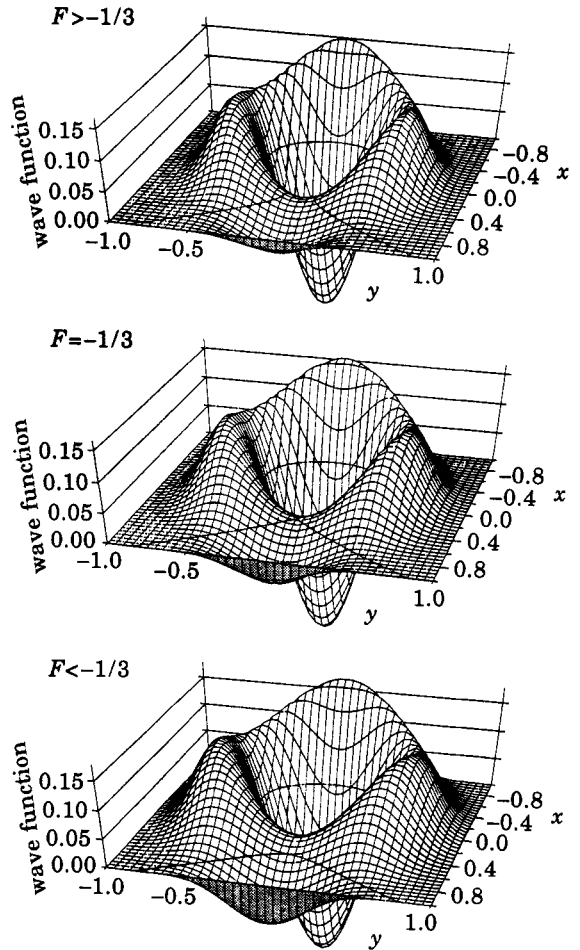Fig. 2. – Plot of the wave function ψ (see table II). Note the zero contour line reproducing the nodes.

exhibiting the nonconservation property is that F, while varying λ, goes through the critical value of $-1/3$. To summarize, we present the potential energy function and its excited eigenfunction of energy E in tables I and II, respectively. In fig. 2 the wave function is drawn for the three different nodal regimes. Figure 3 presents the potential energy function at the critical value $F = -1/3$. No qualitative changes occur at other values of parameter F. Finally, we would like to point out that the solution obtained is a nondegenerate one. To see this, we have performed a careful variational calculation of the lowest eigenvalues by diagonalizing H using a large Hermite-Gaussian basis set. Results are presented in fig. 4. They indicate that the eigenfunction just constructed is nondegenerate (note that a crossing

TABLE I. – *Potential energy function of the coupled anharmonic oscillators:* $V(x, y) = \sum\limits_{i+j \leq 6} c_{ij} x^i y^j$. *Here* $P \equiv F^2 - F/3 + 1/9$.

$$c_{00} = E + \frac{63F}{8P} + \frac{3}{8PF} - \frac{3}{2F} + \frac{1}{2F^2} + \frac{1}{18P^2}$$

$$c_{10} = \frac{21}{2P} + \frac{1}{3PF^2} - \frac{3}{F^2} + \frac{3F}{2P^2} + \frac{1}{9FP^2} - \frac{1}{PF}$$

$$c_{20} = \frac{75}{8PF} + \frac{2}{P^2} + \frac{81F^2}{8P^2} - \frac{27}{2P} + \frac{1}{18P^2F^2} - \frac{1}{PF^2} + \frac{9}{2F^2}$$

$$c_{30} = \frac{3}{2PF^2} + \frac{1}{FP^2} + \frac{27F}{4P^2} - \frac{9}{2PF}$$

$$c_{40} = \frac{63}{8P^2} + \frac{1}{2P^2F^2} - \frac{9}{2PF^2}$$

$$c_{50} = \frac{9}{4P^2F}$$

$$c_{60} = \frac{9}{8F^2P^2}$$

$$c_{02} = \frac{1}{32P^2F^2} - \frac{9}{16P^2} + \frac{81F^2}{32P^2} + \frac{207}{16PF}$$

$$c_{04} = \frac{243}{32P^2} - \frac{27}{32P^2F^2}$$

$$c_{06} = \frac{729}{128F^2P^2}$$

$$c_{12} = \frac{9}{4PF^2} + \frac{3}{4FP^2}$$

$$c_{22} = \frac{243}{16P^2} + \frac{3}{16P^2F^2} - \frac{27}{4PF^2}$$

$$c_{32} = \frac{27}{8P^2F}$$

$$c_{42} = \frac{189}{32F^2P^2}$$

$$c_{24} = \frac{81}{8F^2P^2}$$

of levels of different symmetry, V is invariant under $y \to -y$, occurs just before the critical value) and is the 4th excited state of H in the subspace of even symmetry.

TABLE II. – *Eigenfunction of the coupled anharmonic oscillators:* $P \equiv F^2 - F/3 + 1/9$.

$$\psi(x, y, \lambda) = \left(y^2 - x^2 - Fx - \frac{2}{27} \right) \exp\left[- a_{10}x - a_{20}x^2 - a_{30}x^3 - a_{40}x^4 - a_{02}y^2 - a_{22}x^2y^2 \right]$$

with

$$a_{10} = - \frac{1}{F} - \frac{1}{3P}$$

$$a_{20} = - \frac{9F}{4P} - \frac{1}{6PF} + \frac{3}{2F}$$

$$a_{30} = - \frac{1}{2P}$$

$$a_{40} = - \frac{3}{8PF}$$

$$a_{02} = \frac{1}{8PF} - \frac{9F}{8P}$$

$$a_{04} = - \frac{27}{32PF}$$

$$a_{22} = - \frac{9}{8PF}$$
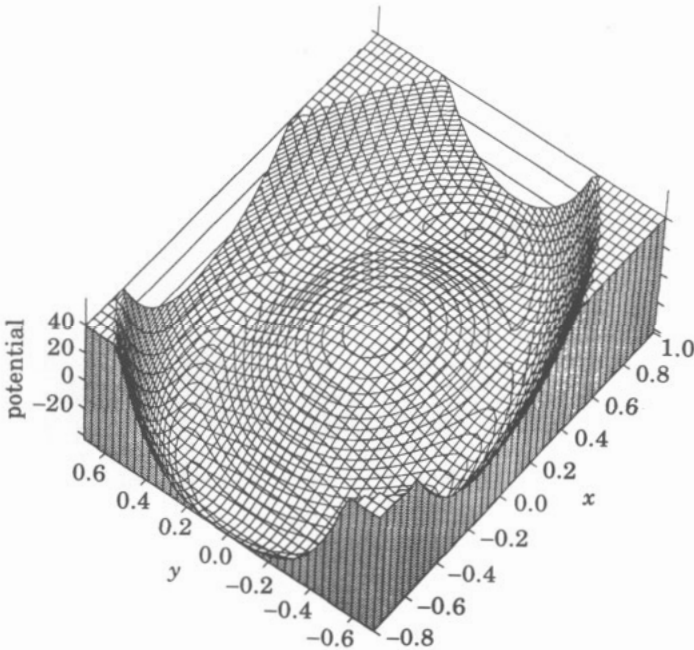
Fig. 3.

Fig. 4.

Fig. 3. – Plot of the potential energy function for $F = - 1/3$. Other values of F give a similar shape.
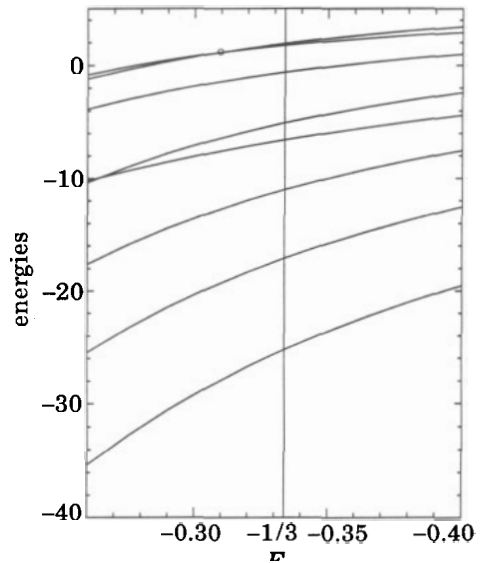
Fig. 4. – Low-lying energies of potential V (table I) *vs.* F (the arbitrary coefficient c_{00} of V being set to zero). The constructed wave function ψ is the 8th level when $F > - 0.31$ and the 7th for smaller values. Crossing of the two energy curves (of different symmetries) is indicated by an open circle.

* * *

REFERENCES

[1] KORSCH H. J., *Phys. Lett. A*, **97** (1983) 77.
[2] COURANT R. and HILBERT D., *Methoden der mathematischen Physik I* (Springer, Berlin) 1930.
[3] UHLENBECK K., *Am. J. Math.*, **98** (1976) 1059.
[4] ALBERT J. H., *Trans. Am. Math. Soc.*, **238** (1978) 341.
[5] PECHUKAS P., *J. Chem. Phys.*, **57** (1972) 5577.
[6] BRÜNING J., *Math. Z.*, **124** (1972) 79.
[7] ROBNIK M., *Phys. Lett. A*, **80** (1980) 117.
[8] ROBNIK M., *J. Phys. A*, **14** (1981) 3195.
[9] BERRY M. V. and WILKINSON M., *Proc. R. Soc. London, Ser. A*, **392** (1984) 15.
[10] BERRY M. V., in *Chaotic Behaviour of Deterministic Systems, Les Houches Summer School Lectures*, edited by R. H. G. HELLEMAN and G. IOOSS, Vol. **36** (North-Holland, Amsterdam) 1983.
[11] GUTZWILLER M. C., in *Chaos in Classical Mechanics* (Springer-Verlag) 1990, Chapt. 15.
[12] CAFFAREL M., CLAVERIE P., MIJOULE C., ANDZELM J. and SALAHUB D. R., *J. Chem. Phys.*, **90** (1989) 990.