The energy levels for a symmetric and nonsymmetric double-well potential in a two-dimensional system using the Hill determinant approach

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Energy levels of the Schrödinger equation for a double-well potential \( V(x, y; Z_x^2, Z_y^2, \lambda) = -Z_x^2 x^2 - Z_y^2 y^2 + \lambda[a_{xx} x^4 + 2a_{xy} x^2 y^2 + a_{yy} y^4] \) in a two-dimensional system are calculated using the Hill determinant approach for several eigenstates and over a wide range of values of the perturbation parameters \((\lambda, Z_x^2, Z_y^2)\). Some of the results calculated by the Hill determinant approach are compared with those results produced by the inner product technique.

1. Introduction

The Schrödinger equation for the one-dimensional double-well potential

\[
V(x; Z^2) = -Z^2 x^2 + x^4
\]

has been the subject of numerous investigations with high calculational accuracy cannot be doubted, and the corresponding literature is abundant [1–7]. These studies have been carried out from both analytical and numerical points of view often in the study of systems for which the potential has been modeled as a double-minimum well, e.g. the ammonia molecule or a hydrogen-bonded solid. Unfortunately most of these investigations have not been extended to multidimensional systems.

In this paper we present extensive numerical calculations which use the Hill determinant technique (in an iterative form) to calculate the energy levels of the Schrödinger equation for a double well potential for a wide range of values of the perturbation parameters \(Z_x^2, Z_y^2, \lambda\) and for several eigenstates.

In this work, the general form of the Schrödinger equation for the double-well potential \( V(x, y; Z_x^2, Z_y^2, \lambda) \) in a two-dimensional system is taken in the form

\[
\left[-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + V(x, y; Z_x^2, Z_y^2, \lambda)\right] \psi_{n_x,n_y}(x, y) = E_{n_x,n_y} \psi_{n_x,n_y}(x, y),
\]

where \( V(x, y; Z_x^2, Z_y^2, \lambda) \) is given as
\[ V(x, y; Z_x^2, Z_y^2, \lambda) = -Z_x^2x^2 - Z_y^2y^2 + \lambda [a_{xx}x^4 + 2a_{xy}x^2y^2 + a_{yy}y^4] . \] (3)

The eigenvalue spectrum of the Schrödinger equation (2) with \( V(x, y; Z_x^2, Z_y^2, \lambda) \) has the feature that the lower eigenvalues for states \( E_{00}, E_{11}, \) and \( (E_{01} = E_{10}) \) are closely bunched together if the values of \( Z_x^2 \) and \( Z_y^2 \) are sufficiently large at small values of \( \lambda \). As \( Z_x^2 \) and \( Z_y^2 \) increase, the magnitude of the splitting between these levels decreases i.e. \( |E_{11} - E_{00}| \approx 0 \) or \( |E_{01} - E_{00}| \approx 0 \). These energy levels are shown in figs. 1 and 2.

The depth of the double well is controlled by the parameters \( Z_x^2, Z_y^2 \) at constant value of the perturbation parameters \( (\lambda, a_{xx}, a_{xy}, a_{yy}) \) (see fig. 3). The Hill determinant approach works well for small and medium values of \( Z_x^2, Z_y^2 \) at small values of \( \lambda \); as \( Z_x^2 \) and \( Z_y^2 \) increase the depth of the well increases and for deep wells the degree of convergence decreases.

Our work illustrate the high flexibility of the Hill determinant approach; this gives it an advantage over the inner product technique, which can only work for small values of \( Z_x^2 \) and \( Z_y^2 \), at which the potential minima are shallow [8].

Since many of our results for this problem are not available in the literature it was found useful to check them using another method of calculation such as the inner product technique. The agreement in the results calculated by two different methods suggests accuracy yielded by our calculations is good (see table 4).

For purposes of clarity, this paper is divided into three sections. Section two is concerned with the Hill determinant approach and its use to calculate the energy eigenvalues for double well potential, and section three contains a discussion of the results.

Fig. 1. Graph of three energy levels for different values of \( Z^2 \) for the case \( a_{xx} = a_{yy} = 1, a_{xy} = 0 \); at \( Z_x^2 = Z_y^2 = Z^2 \) and \( \lambda = 1 \).