International Journal of Theoretical Physics, Vol. 41, No. 1, January 2002 (© 2002)

Quantum Monodromy in the Spectrum of Schrödinger Equation With a Decatic Potential

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Received March 16, 2001

In this study the spectral problem of the two-dimensional Schrödinger equation with the cylindrically symmetrical decatic potential is carried out. The concept of quantum monodromy is introduced to give insight into the energy levels of system with this potential. It is shown that quantum monodromy occurs at $\rho = 0$ in the distribution of eigenstates around a critical point on the spectrum at $E = 0$ with zero angular momentum, such that there can be no smoothly valid assignment of quantum number. Cases with the three-well and four-well potentials are presented to give rise to the double degeneracies with respect to energy except for the angular momentum $m = 0$.

1. INTRODUCTION

One of the important tasks of quantum mechanics is to solve the Schrödinger equation with the physical potentials. The anharmonic potentials have played an important role in the evolution of many branches of physics. Generally, it has been realized that many interesting and important features of numerous systems come from the anharmonic character of their vibrations. During the past several decades, many efforts have been produced to study the stationary Schrödinger equation with the anharmonic potentials (Bose, 1994; Bose and Varma, 1990; Calogero, 1967; Coleman, 1988; Dong, 2000, 2001a,b; Dong *et al.*, 1999; Dong and Ma, 1998; Emin, 1982; Emin and Holstein, 1976; Esposito, 1998a,b, 2000; Hashimoto, 1979, 1980; Kaushal, 1989, 1991; Kaushal and Parashar, 1992; Newton, 1967; Özcelik and Simsek, 1991; Reid, 1970; Share and Behra, 1980; Simsek and Özcelik, 1994; Znojil, 1982a,b, 1989, 1990). For example, the anharmonic oscillator with quartic anharmonicity in the potential has been widely discussed at both the classical and quantum mechanical limits of the theory under the case of one-dimensional and two-dimensional spaces (Bender and Wu, 1973; Hoie *et al.*, 1978; Jaenicke and

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Kleinert, 1993; Karrlein and Kleinert, 1988; Langer, 1967; Simon, 1970). Case with the sextic potential has been also studied extensively (Child, 1998; Dutta and Willey, 1988; Klauder, 1965; Pan *et al.*, 1999; Singh *et al.*, 1990; Tater, 1987; Turbiner, 1988a,b; Znojil, 1982a,b). Up to recently, it has been seen that a very interesting physical phenomenon known as the quantum monodromy (Bates, 1991; Child, 1998; Child *et al.*, 1999, 2000; Cushman, 1983; Cushman and Sadovskii, 1999; Hazewinkei, 1994; Marsden and Hoffman, 1987; Ngoc, 1999; Sadovskii and Zhilinski, 1999; Solari *et al.*, 1996) occurs in the eigenvalue distribution around a critical point in the joint spectrum at $(E, m) = (0, 0)$ under the case of champagne bottle potential. It is surprising that the idea of the quantum monodromy had been dormant for many years before the new interest led to the experiment discovery in the spectrum of excited water molecules (Child *et al.*, 1999). The purpose of this work is to address the special feature with quantum monodromy of the decatic potential, which has never been addressed in the literature, to our knowledge.

The term monodromy (meaning "once round") used in this note stems from the mathematical literature (Hazewinkei, 1994; Marsden and Hoffman, 1987). One kind of physical application occurs in any time-periodic system, where for example the stabilities of fixed points in the period map are characterized by the eigenvalues of the monodromy matrix (Solari *et al.*, 1996). Another kind of application comes from the classical and mechanical literature (Marsden and Hoffman, 1987; Solari *et al.*, 1996), where it is applied to demonstrate a gross topological obstruction to the global construction of angle-action variables. From the viewpoint of the quantum mechanics, this implies the absence of any smooth valid set of quantum numbers for the entire spectrum. Quantum correspondences have been demonstrated for a champagne bottle model (Child, 1998; Child *et al.*, 2000) and for the molecular spectrum of H_2O (Child *et al.*, 1999). The same characteristic energy pattern are demonstrated below for the decatic potential. Moreover, it is found that the double degeneracies with respect to the energy occurs in the case of the three-well and four-well potentials. Special cases with the four-well potential are also shown to arise quantum monodromy.

This paper is organized as follows. The eigenvalues of the Schrödinger equation with the decatic potential obtained by a full variational method is given in section 2. Section 3 is devoted to a demonstration and discussion of the quantum monodromy. A concluding remark is given in the final section 4.

2. THE QUANTUM-MECHANICAL SPECTRUM

As we know, the variational method used in this note has been widely applied to the different fields of physics and chemistry. Natural units $\hbar = c = 1$ are used throughout this paper, if not explicitly stated otherwise. Considering the two-dimensional Schrödinger equation with a potential $V(\rho)$ that depends only on the distance ρ from the origin, the quantum-mechanical Hamiltonian can be written as

$$\left[-\frac{1}{2}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}\right)+\frac{m^2}{\rho^2}-V(\rho)\right]\psi(\rho)=E\psi(\rho) \tag{1}$$

where $V(\rho)$ is the decatic potential

$$V(\rho)=a\rho^2+b\rho^4+c\rho^6+d\rho^8+f\rho^{10}.$$

The numerically accurate eigenvalues are easily obtained by an expansion in normalized degenerated harmonic oscillator states

$$\psi(\rho)=\sum_n c_n R_{n,m}(\rho) \tag{2}$$

where

$$R_{n,m}(\rho)=\left[\frac{2((n-m)/2)!}{((n+m)/2)!}\right]^{1/2}\rho^m L^{m}_{\frac{n-m}{2}}(\rho^2) \tag{3}$$

in which $L^{\alpha}_{\nu}(z)$ is the associated Laguerre polynomial (Abramowitz and Stegun, 1994). The necessary matrix elements follow from the recurrence relations

$$2\hat{k}R_{n,m}=\frac{1}{2}[(n+2)^2-m^2]^{1/2}R_{n+2,m}+(n+1)R_{n,m}+\frac{1}{2}[n^2-m^2]^{1/2}R_{n-2,m} \tag{4}$$

where

$$\hat{k}=-\frac{1}{2}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)-\frac{m^2}{\rho^2}\right] \tag{5}$$

and

$$\rho^2R_{n,m}=-\frac{1}{2}[(n+2)^2-m^2]^{1/2}R_{n+2,m}+(n+1)R_{n,m}-\frac{1}{2}[n^2-m^2]^{1/2}R_{n-2,m} \tag{6}$$

from which, we can easily obtain the terms in ρ^4, ρ^6, and ρ^8 as

$$\begin{aligned}\rho^4R_{n,m}=&\ \frac{1}{4}[((n+2)^2-m^2)((n+4)^2-m^2)]^{1/2}R_{n+4,m}-(n+2)\\ &\times[(n+2)^2-m^2]^{1/2}R_{n+2,m}+\frac{1}{2}[(1-m^2)\\ &+3(1+n)^2]R_{n,m}-n[n^2-m^2]^{1/2}R_{n-2,m}\\ &+\frac{1}{4}[(n^2-m^2)((n-2)^2-m^2)]^{1/2}R_{n-4,m}\end{aligned} \tag{7}$$

and

$$\begin{aligned}
\rho^6 R_{n,m} = & -\frac{1}{8}[((n+2)^2-m^2)((n+4)^2-m^2)((n+6)^2-m^2)]^{1/2} R_{n+6,m} \\
& + \frac{3(n+3)}{4}[((n+2)^2-m^2)((n+4)^2-m^2)]^{1/2} R_{n+4,m} \\
& - \frac{3}{8}[5(n+2)^2-m^2+4][(n+2)^2-m^2]^{1/2} R_{n+2,m} \\
& + \frac{1}{2}[(1+n)(12-3m^2+10n+5n^2)] R_{n,m} \\
& - \frac{3}{8}[5n^2-m^2+4][n^2-m^2]^{1/2} R_{n-2,m} + \frac{3(n-1)}{4} \\
& \times [((n-2)^2-m^2)(n^2-m^2)]^{1/2} R_{n-4,m} - \frac{1}{8}[((n-4)^2-m^2) \\
& \times ((n-2)^2-m^2)(n^2-m^2)]^{1/2} R_{n-6,m}
\end{aligned} \tag{8}$$

also

$$\begin{aligned}
\rho^8 R_{n,m} = & \frac{1}{16}[((n+2)^2-m^2)((n+4)^2-m^2)((n+6)^2-m^2) \\
& \times ((n+8)^2-m^2)]^{1/2} R_{n+8,m} - \frac{n+4}{2}[((n+2)^2-m^2) \\
& \times ((n+4)^2-m^2)((n+6)^2-m^2)]^{1/2} R_{n+6,m} + \frac{1}{4}[7(n+3)^2 \\
& - m^2+9][((n+2)^2-m^2)((n+4)^2-m^2)]^{1/2} R_{n+4,m} \\
& - \frac{n+2}{2}[7(n+2)^2-3m^2+20][(n+2)^2-m^2]^{1/2} R_{n+2,m} \\
& + \frac{1}{8}[192+3m^4+400n+340n^2+140n^3+35n^4 \\
& - 30m^2(2+2n+n^2)] R_{n,m} - \frac{n}{2}(7n^2-3m^2+20) \\
& \times [n^2-m^2]^{1/2} R_{n-2,m} + \frac{1}{4}[7(n-1)^2-m^2+9][((n-2)^2-m^2) \\
& \times (n^2-m^2)]^{1/2} R_{n-4,m} + \left(1-\frac{n}{2}\right)[((n-4)^2-m^2)((n-2)^2-m^2) \\
& \times (n^2-m^2)]^{1/2} R_{n-6,m} + \frac{1}{16}[(n^2-m^2)((n-2)^2-m^2) \\
& \times ((n-4)^2-m^2)((n-6)^2-m^2)]^{1/2} R_{n-8,m}
\end{aligned} \tag{9}$$

and terms in ρ^{10} can be also obtained and need not be expressed explicitly for simplicity.

The numerical convergence with respect to truncation of the resulting tridiagonal matrix depends on the parameters of the decatic potential. In the following section, we will discuss the results obtained by this method.

Besides, as discussed in Child *et al.* (2000), there exists the hidden symmetry for the sextic physical potential $V(r) = ar^2 + br^4 + cr^6$. The system studied in this note will also imply hidden symmetry since the structure of decatic physical potential is similar to that of sextic physical potential. For example, it is noted that the substitution $\rho \to i\rho$ reverse the sign of b and d and E in (1), leaving the remaining parameters invariant.

3. QUANTUM MONODROMY

This work on quantum monodromy is largely addressed in semiclassical terms (Bates, 1991; Child, 1998; Child *et al.*, 1999, 2000; Cushman, 1983; Cushman and Sadovskii, 1999; Hazewinkei, 1994; Marsden and Hoffman, 1987; Ngoc, 1999; Sadovskii and Zhilinski, 1999; Solari *et al.*, 1996). In Fig. 1, the points mark the numerically determined eigenvalues around $E = 0$ for angular momentum $-30 < m < 30$. To bring out the underlying patterns, the full and broken lines are used to join points with a common radial quantum number ν and a common total quantum number $n = 2\nu + |m|$, respectively. It is found that ν quantized curves shows a sharp transition from smooth variation through $m = 0$ when $E < 0$, to a discontinuous first derivative when $E > 0$. However, the opposite is true for the broken n quantized curves. Nonanalyticity in the relevant action integral is responsible for the dislocation in each case. The dislocations also have consequences for the parallel transport around the origin of any vector on the lattice of quantum numbers. As show elsewhere (Bates, 1991; Child *et al.*, 1999) any vector $(\Delta m, \Delta n)$ returns to $(\Delta m', \Delta n')$ such that

$$\begin{pmatrix} \Delta m' \\ \Delta n' \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \Delta m \\ \Delta n \end{pmatrix}$$

because the parallel transport entails a switch from one sheet of the classical action integral to the next (Child *et al.*, 1999).

The corresponding champagne bottle potential is illustrated in Fig. 2.

In this case, the parameters of the given potential are taken as $a = -10$, $b = 0.1$, $c = 0.01$, $d = 0.001$, and $f = 0.00001$, respectively. In fact, there will exist such a phenomenon as quantum monodromy only if the potential is taken as the champagne bottle potential.

Furthermore, the three-well and four-well potential can be also obtained by taking the suitable parameters and illustrated in Figs. 3 and 4, respectively.

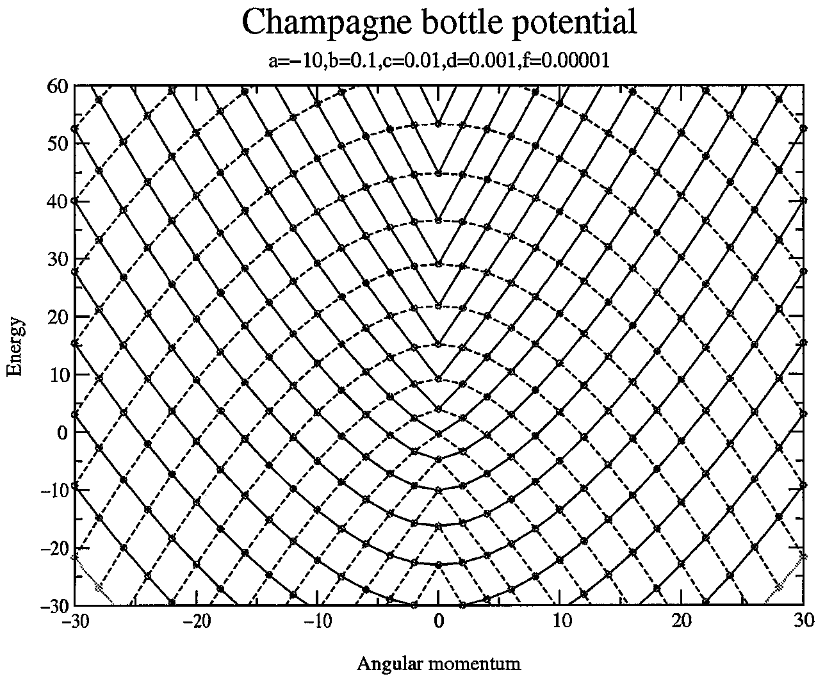

Fig. 1. The full and broken lines join points with the radial quantum number ν and the "total" quantum number $n = 2\nu + m$ values, respectively. The parameters of the potential are taken as $a = -10$, $b = 0.1$, $c = 0.01$, $d = 0.001$, and $f = 0.00001$, respectively.

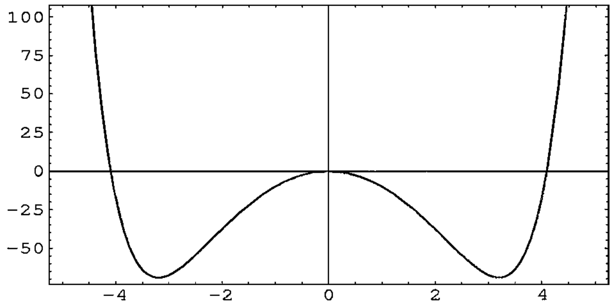

Fig. 2. The parameters of the potential are taken as $a = -10$, $b = 0.1$, $c = 0.01$, $d = 0.001$, and $f = 0.00001$. The abscissa denotes the radial ρ and the ordinate denotes the value of the potential.

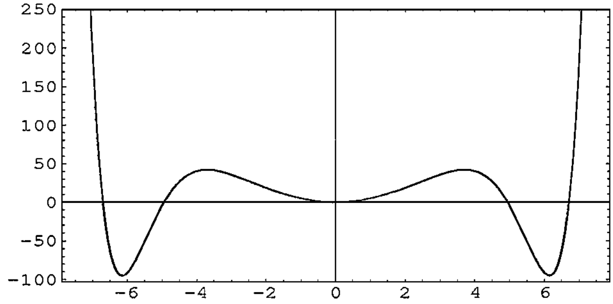

Fig. 3. The parameters of the potential are taken as $a = 5, b = -0.1, c = 0.002, d = -0.0005$, and $f = 0.00001$. The abscissa denotes the radial ρ and the ordinate denotes the value of the potential.

For the triple well potential, the corresponding parameters are taken as $a = 5, b = -0.1, c = 0.002, d = -0.0005$, and $f = 0.00001$, respectively, it is shown from Fig. 5 that the double degeneracies with respect to energy occurs except for $m = 0$.

For the four-well potential, the corresponding parameters are taken as $a = -22, b = 1.25, c = 0.008, d = -0.001$, and $f = 0.00001$, respectively. It is also shown that double degeneracies occur. Moreover, it is found that quantum monodromy also occurs under the case of the four-well potential. This can be explained by Fig. 6, from which it is shown to exist a champagne bottle potential so that this kind of phenomenon is not surprising. It is also found from Fig. 5 that the total quantum number n changes discontinuously, so does the radial quantum number ν. Certainly, the parameters are taken arbitrarily. The purpose of taking such parameters into consideration is to make the problem clear and simple. The special cases for $d = f = 0$ and $c = d = f = 0$ have been carried out in Child

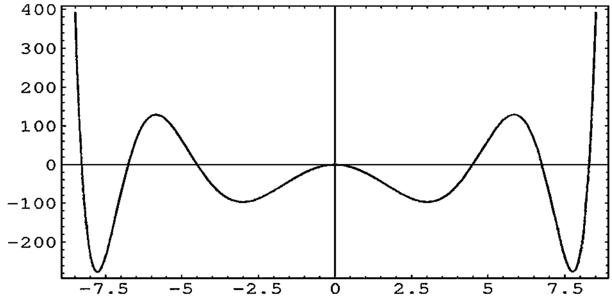

Fig. 4. The parameters of the potential are taken as $a = -22, b = 1.25, c = 0.008, d = -0.001$, and $f = 0.00001$. The abscissa denotes the radial ρ and the ordinate denotes the value of the potential.

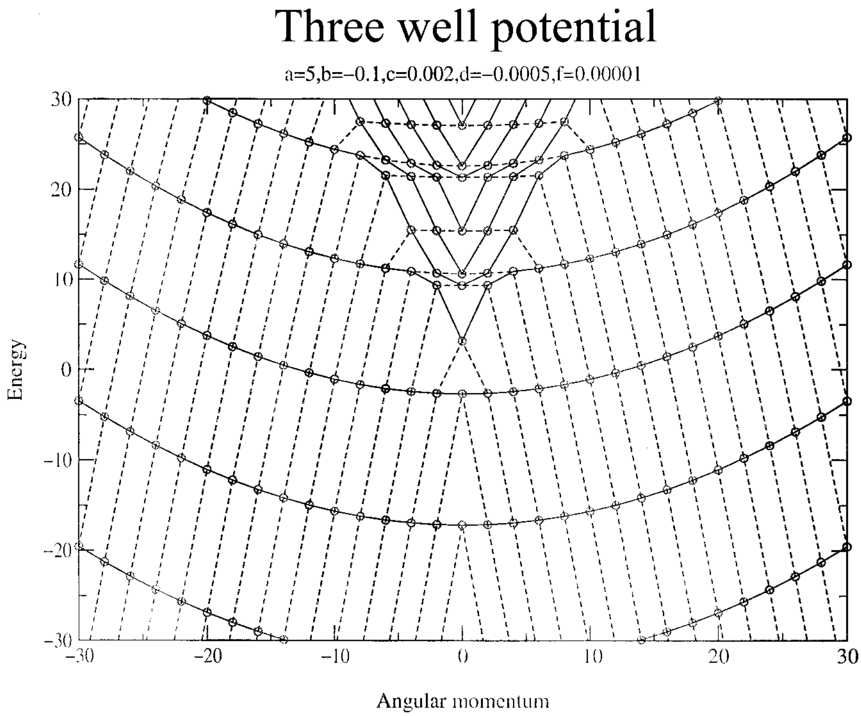

Fig. 5. The full and broken lines join points with the radial quantum number ν and the "total" quantum number $n = 2\nu + m$ values, respectively. The parameters of the potential are taken as $a = -22$, $b = 1.25$, $c = 0.008$, $d = -0.001$, and $f = 0.00001$, respectively.

(1998) and Child *et al.* (2000), respectively. However, the study of the single well potential is beyond our interest.

Actually, the case of champagne bottle potential illustrated in Fig. 2 looks like that studied in Child (1998) and Child *et al.* (2000) except for the different power of the variable ρ. In fact, it is not surprised at the case with negative a and positive b, c, d, f with the property of the champagne bottle because the contribution from these terms plays the same role as that with negative a and positive b studied in Child (1998) and that with negative a, b and positive c discussed in Child *et al.* (2000).

4. CONCLUDING REMARKS

In this paper, the quantum-mechanic spectrum of the two-dimensional Schrödinger equation with the decatic potential $V(\rho) = a\rho^2 + b\rho^4 + c\rho^6 + d\rho^8 + f\rho^{10}$ is obtained by variational method. On taking the suitable parameters of the given potential, it is shown that quantum monodromy occurs at $r = 0$ in the

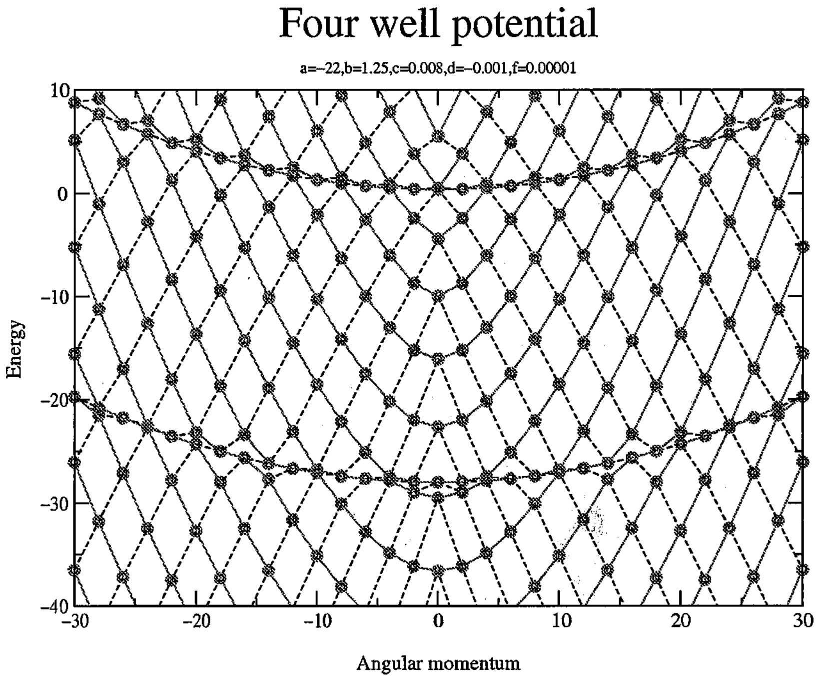

Fig. 6. The full and broken lines join points with the radial quantum number ν and the "total" quantum number $n = 2\nu + m$ values, respectively. The parameters of the potential are taken as $a = -22$, $b = 1.25$, $c = 0.008$, $d = -0.001$, and $f = 0.00001$, respectively.

distribution of eigenstates around a critical point on the spectrum at $E = 0$ with zero angular momentum. Cases with the triple-well and four-well potentials are shown to give rise to the double degeneracies with respect to energy except for $m = 0$. Also, it is found that the radial quantum number ν and the total quantum number n change discontinuously, especially case with the four-well potential also exists the quantum monodromy, which is determined by the nature of the champagne bottle potential illustrated by Fig. 6. As discussed above, we have however stressed the generality of the abrupt change in level structure about the monodromy point, for all systems with cylindrically symmetric potential barriers. It remains to be seen whether this interesting phenomenon known as the quantum monodromy occurs in other anharmonic physical potential.

ACKNOWLEDGMENTS

The author thanks Prof M. S. Child for drawing attention to this interesting system and for invitation to University of Oxford where the collaboration and discussion took place. S. H. Dong thanks Prof A. Frank for invitation to Universidad Nacional Autonoma de Mexico. This work is supported in part by the Royal Society of London and in party by CONACyT, Mexico, under project 32397-E.

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