Miller-Good Method for Symmetric Double Potential Wells

Luis Alberto del Pino*

*Also at Departamento de Física, Facultad de Montaña, Universidad de Pinar del Río, Cuba

Instituto de Física, Universidad de Guanajuato
León, Guanajuato, México.

and

Hipólito Mena

Departamento de Física, Facultad de Montaña,
Universidad de Pinar del Río, Pinar del Río, Cuba

January 14, 2018

Abstract

The ground state energy of the quartic anharmonic oscillator is calculated by employing the Miller-Good method. For this purpose an extension of the procedure is developed which is suitable for considering four turning points situations. A criterion for the selection of the auxiliary quantum mechanical problem is also advanced.
1 Introduction

In many physical situations of interest, quantum mechanical particles move under the action of potential having various minimal points. A relevant one of this problems is the oscillatory movement of the Nitrogen molecule between both sides of the hydrogenic triangle in the ammonia molecule. Numerous models and methods for their solutions have been proposed for this system [1] [2] [3] [4].

A main objective of the present work is to illustrate a way to extended the Miller Good (MGM) method for the WKB studies of symmetric double wells by exploiting the symmetry properties [5]. The extension is obtained by proposing a modification of the calculation scheme of the method. In addition a criterion for the appropriate selection of the auxiliary quantum mechanical problem is also introduced. The procedure is here applied to the calculation of the ground state energy of the quartic anharmonic oscillator. Within the range of the parameters in which the technique is applicable the calculated values give satisfactory estimates of the ground state energy. In particular they improve the predictions of another approximate approach recently proposed in the literature [6], and gives numerical results of similar quality that the ones presented in [7].

2 Extension of the Miller-Good Method

The calculation scheme of the Miller-Good (MGM) method is described as follows [5]. As a solution for

\[ \psi''(x) + \frac{p^2(x)}{\hbar^2} \psi(x) = 0 \]  

where \( p(x) = 2m \sqrt{E - v(x)} \), the following change of variables is proposed

\[ \psi(x) = \frac{1}{\sqrt{s'(x)}} \phi[s(x)] \]  

where \( \phi \) is a known solution of the auxiliary quantum mechanical problem:
\[ \phi''(s) + \frac{P^2(s)}{\hbar^2} \phi(s) = 0 \]  

(3)

defined by the also known function \( P \), and the function \( s \), which establishes the link between the original problem and the auxiliary. The function \( s \) in order to furnish the mentioned equivalence satisfies the equation:

\[ P^2(s)s'' = p^2(x) + \hbar^2 D_s(x) \]  

(4)

\[ D_s(x) = \frac{3}{2} s''^2 - \frac{1}{2} \frac{s'''}{s'} \]  

(5)

Up to this point, the transformation is exact. The Miller-Good approximation consists in disregard the expression \( D \) defined by (5) in the equation for \( s \) given in (4). This approximation, then, produces the following solution for the wave-function

\[ \psi_{M-G} = \frac{1}{\sqrt{|s_0(x)|}} \phi[s_0(x)] \]  

(6)

in which \( s_0 \) is determined from the equation:

\[ P(s_0)s_0' = p(x), \]  

(7)

the boundary conditions:

\[ s_0(x_1) = s_{01} \]  

(8)

where \( x_1 \) is a turning point, and the integral condition

\[ \int_{s_{01}}^{s_{02}} ds_0 P(s_0) = \int_{x_1}^{x_2} dx p(x) \]  

(9)

The last expression constitutes the Miller-Good quantization rule which coincides with the known WKB rule if in the quality of the auxiliary problem defining function is selected \( P(s) = \hbar^2(\alpha - s^2) \) with \( \alpha = 2n + 1 \).
However, a general criterion for selecting the auxiliary problem in each concrete situation is lacking. Only qualitative guides supported by the experience are at hand. It is an aim in this work to introduce a modification of the approximation scheme just presented allowing to appropriately select the auxiliary problem in a general way which adjust relevant characteristics of the considered task.

For the above mentioned purpose, let us perform in (1) the transformation $x = x(y)$ through which this equation becomes

$$
\frac{\psi''}{x'^2} - \frac{x''}{x^3} \psi' + \frac{p^2(y)}{h^2} \psi = 0 \quad (10)
$$

Assuming now that the equation

$$
\phi''(s) + \frac{p^2(s)}{h^2} \phi(s) = 0 \quad (11)
$$

have a known exact solution and that this system have: the same number of turning points which are coincident the original ones, coinciding asymptotic behavior in relevant regions, etc.. Then, the here proposed general rule consists in to adopt such a problem defined by (11) as the auxiliary one. In this case, the condition which the function $s$ should obey for assuring the equivalence of the auxiliary problem (11) with the original one in the form (10) is given by:

$$
p^2(s)s''(y) = x''(y)p^2(y) + h^2[D_s(y) - D_{s,x}(y)] \quad (12)
$$

$$
D_{s,x} = \frac{3}{2} \frac{s''}{s'x'} - \frac{1}{2} \frac{x'''}{x'} \quad (13)
$$

Again in the order zero approximation consisting in disregard the $D$ function in the equation for $s$ it follows:

$$
p(s_0)'(y) = x'(y)p(y) \quad (14)
$$

and the initial and boundary conditions

$$
s_0(y_1) = s_{01} \quad (15)
$$
\[
\int_{s_{01}}^{s_{02}} ds_0 p(s_0) = \int_{y_1}^{y_2} dy x'(y) p(y)
\]  
(16)
in which \(s_{01}, s_{02}\) and \(y_1, y_2\) are the turning points in the variables \(s\) and \(y\) respectively.

The proposed transformation of the method not only allows to select the auxiliary problem in an adequate manner, but also permits to extend the Miller-Good method to systems having four turning points. Let us suppose that the inverse of the initial transformation \(x(y)\) used for construct the auxiliary problem became even. Then, if the potential is also an even function of \(x\), the same symmetry is guaranteed for the function \(s_0\) with respect to \(x\). This property allows to select as the auxiliary problem the one corresponding to two isolated wells.

3 Ground State Energy of the Quartic Anharmonic Oscillator

In this ending section, the application of the technique to the calculation of the ground state energy of the one particle quantum mechanical problem defined quartic anharmonic potential

\[
v(x) = \lambda x^4 - \frac{m\omega^2}{2} x^2, \quad E < 0
\]  
(17)

The \(x(y)\) transformation having the required characteristic is given by:

\[
\frac{x^2}{x_0^2} = y + \frac{1}{2}
\]  
(18)

\[
x_0 = \sqrt{\frac{m\omega^2}{2\lambda}}
\]  
(19)

After this transformation, the \(p\) function defining the auxiliary problem (11) takes the form \(p^2(s_0) = \hbar^2(\alpha - s_0^2), \alpha = 2n + 1\) and the equation (12) becomes

\[
(1 - \xi^2)\xi^2 = 2 \frac{z^4}{\alpha^2 \lambda^2} \frac{1 - \eta^2}{1 + 4z\eta} + \frac{1}{\alpha^2} D\xi(\eta) + \frac{4z^2}{\alpha^2} D\eta
\]  
(20)
\[ D_{\eta \xi} = \frac{3\xi''}{2z\xi'(1+4z\eta)} + \frac{3}{2(1+4z\eta)} \] (21)

\[ \xi^2 = \frac{s^2}{\alpha} \] (22)

\[ \eta = \frac{y}{2z} \] (23)

\[ \lambda' = \frac{\hbar\lambda}{m^2\omega^3} \] (24)

The ground state energy in the zero order approximation, as following from (16) satisfies the two coupled equations

\[ E = \frac{\hbar\omega}{\lambda'} \left( z^2 - \frac{1}{16} \right) \] (25)

\[ \frac{\pi}{2} = \sqrt{z^2} \frac{2}{\lambda'} \int_{-1}^{1} \sqrt{1 - \frac{\eta^2}{1 + 4z\eta}} d\eta \] (26)

\[ z < \frac{1}{4} \] (27)

In order to qualitatively evaluate the nature of the results of the method as applied to this problem, let us note that inside one of the wells, an approximate solution of the equation

\[ \sqrt{1 - \xi^2} \xi' = \sqrt{2} z \frac{\eta^2}{\lambda'} \sqrt{1 - \frac{\eta^2}{1 + 4z\eta}} \] (28)

\[ \xi(-1) = -1 \] (29)

becomes \( \xi = \eta \), for values of \( z << \frac{1}{4} \). After substituting this solution in (20) it follows that this terms is order \( z^2 \), a fact which indicates that performed approximation should be valid for small values of \( z \).

The Figure 1 below presents the results for the calculation of the ground state energy for various values of the parameter \( \lambda' \), as evaluated from equations (25) y (26). Also reported are the energy values of the exact solution, and the results of the calculation reported in [6] following the method proposed in that work. As it can be observed the results of the treatment improve for small values of \( z \) and remains working well up to values corresponding to ground state energies being a half of the deepness of the well. In Table the
numerical results used for the graphical picture are given.

**Table 1**

| $\lambda'$ | $z^2$   | $\frac{E}{h\omega}$ | $\frac{E}{h\omega}$ (exact) | $\frac{E}{h\omega}$ [1] |
|------------|---------|-----------------------|-----------------------------|------------------------|
| 0.01       | 0.0069  | -5.55                 | -                           | -                      |
| 0.02       | 0.0138  | -2.43                 | -2.43                       | -2.99                  |
| 0.025      | 0.0167  | -1.83                 | -1.82                       | -1.88                  |
| 0.03       | 0.02    | -1.41                 | -                            | -                      |
| 0.035      | 0.0233  | -1.12                 | -1.12                       | -1.00                  |
| 0.04       | 0.0272  | -0.88                 | -                            | -                      |
| 0.05       | 0.0345  | -0.56                 | -0.63                       | -0.50                  |
| 0.06       | 0.0412  | -0.35                 | -                            | -                      |
| 0.07       | 0.0492  | -0.19                 | -                            | -                      |
| 0.075      | 0.0523  | -0.13                 | -0.30                       | -0.26                  |
| 0.08       | 0.0568  | -0.07                 | -                            | -                      |
| 0.085      | 0.0593  | -0.03                 | -0.23                       | -0.20                  |
| 0.09       | 0.0610  | -0.016                | -                            | -                      |
| 0.1        | 0.0612  | -0.013                | -0.15                       | -0.13                  |
4 Conclusions

An extension of the Miller-Good method is proposed. The approach can be applied to symmetric double potential well problems. For this purpose, it is sufficient to find the transformation allowing to transform the double well in two isolated wells. The numerical results of the application of the method to the quartic anharmonic potential shows that the approach works well in regions where other method fails [6]. The quasi classical character of the approximation indicates the possibility for that, in general, the extension proposed become useful in the region of small values of the transmission coefficient through the barrier. This affirmation is supported by the fact that the results shown in Table 1 are satisfactory ones for the small, values of $\lambda'$ implying also small values for the transmission coefficients. It is need to remark that the calculation within the proposed approach can be improved by using a better value of the parameter $\alpha$ calculated from the exact solution of an improved auxiliary problem. The useful modification consists in extending the auxiliary potential to be an even function with respect to the point $y = -1/2$. An approximated solution of this task have been obtained in Ref. [4].

5 Acknowledgements

We express our deep gratitude to our former advisor Dr. Igropulos which introduced us to this field of activity. We also would like to extend this gratitude to the members of the Group of Theoretical Physics of ICIMAF, in particular to Drs. Alejandro Cabo, Aurora Perez, Augusto Gonzalez and Lic. David Oliva, for their advise and collaboration. The support of CONACyT and the warm hospitality of the Institute of Physics for the Guanajuato University, where this work was finished, are also greatly appreciated.

References

[1] J.D. Swalen and J.A. Ibers. J. Chem. Phys. 36 (1961) 1914.
[2] R.R. Newton and L.H. Thomas. J. Chem. Phys. 16 (1948) 310.
[3] M.F. Manning. J. Chem. Phys. 3 (1935) 136.

[4] F.T. Wall and George Glocker. Journal of Chemical Physics 5 (1937) 314.

[5] F. Galindo et. al., Mecanica Cuantica, Editorial Reverte, Madrid (1977).

[6] N. Aquino, J.L. Lopez-Bonilla and M.A.Rosales, Rev. Mex. Fis. 40 (1994) 946.

[7] C.S. Park, S.Y. Lee, J.R. Kahng, S.K. Yoo, D.K. Park, C.H.Lee and E.S. Ying, Los Alamos Preprint Archive, quant-ph/9609008 (9 Sept. 1996).