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Path integral treatment of the deformed Schiöberg-type potential for some diatomic molecules

Assia Amrouche, Ahmed Diaf, and Mohammed Hachama

Abstract: The bound state solution of the Feynman propagator with the deformed generalized Schiöberg potential is determined using an approximation of the centrifugal term. The energy eigenvalue expression is computed using Duru-Kleinert space-time transformation for both positive and negative deformation parameters of diatomic molecules. Besides, the rotation-vibration energy eigenvalues are numerically calculated for some diatomic molecules and compared with those given in the literature. The obtained results are in agreement with those given by state-of-the-art approximate and numerical methods.

Key words: Path integral, deformed Schiöberg-type potential, $l-$states.

1. Introduction

The study of analytical solutions for empirical potential functions of diatomic molecules has been the object of many investigations for several reasons. For instance, in chemical physics [1], an accurate potential energy curve is needed in the evaluation of spectroscopic constants and reactive scattering theoretical studies. In addition, accurate vibrational energies and wave functions are required in studies such as the vibrational excitation of electron-molecule collision which involves molecular vibrational excitation process.

Several potential functions has been proposed in the literature. A first simple empirical analytical potential function was proposed by Morse [2] and has been employed in a wide variety of problems in chemical physics such as in molecular spectroscopy [3] and in molecular dynamics simulation [4]. Another famous hyperbolic type potential is the Schiöberg potential [5] which includes the Morse, Kratzer and Coulomb potentials as special cases. More general potential functions have been constructed by Eğrifes et al. [10, 11, 12], based on the deformed hyperbolic functions [9], and which are identical to the Tietz potential model for diatomic molecules [13, 14]. These q-deformed potentials have been widely used in different applications such as the quantum statistical theory [15], the conformal field theory [16, 17], the nuclear structures [18], and the chemical physics [19]. For the above potentials, the Schrödinger's equation has been exactly solved for the s-states. For $\ell \neq 0$ states, several approximate techniques have been proposed. We can cite the Nikiforov-Uvarov method [6], the function analysis [7], the asymptotic iteration [8], and the Feynman path integrals [24, 25, 26]. In recent papers, some q-deformed empirical potentials have been addressed, such as Woods-Saxon [20], the four-parametric deformed Schiöberg type [21, 22] and the q-deformed hyperbolic Poschl-Teller potential [23].

Recently, Mustafa introduced a four-parametric deformed Schiöberg-type potential for diatomic molecules [21]. He computed the energy spectrum of the $\ell-$states using the super-symmetric quantization in the Schrödinger framework. In this paper, we use the Feymann path integral formalism to solve this potential. In Section 2, we discuss the deformed Schiöberg-type potential and show some properties. In Section 3, the Feynman propagator is investigated using the Duru-Kleinert method to obtain the energy eigenvalues. In Section 4, numerical results for some diatomic molecules are given and compared with previous ones [21, 27]. Finally, some concluding remarks are given in Section 5.

2. The Schiöberg-type potential

Based on the original expression of the Schiöberg potential [5], Mustafa [21] has proposed the four-parametric deformed Schiöberg-type potential:

$$U(r) = A\left[B + \tanh_q(\alpha r)\right]^2, \tag{1}$$

where the $q-$deformation of the usual hyperbolic functions are defined by the following expressions:

$$\begin{aligned}
\tanh_q(\alpha r) &= \frac{\sinh_q(\alpha r)}{\cosh_q(\alpha r)}, \\
\sinh_q(\alpha r) &= \frac{e^{\alpha r} - q e^{-\alpha r}}{2}, \\
\cosh_q(\alpha r) &= \frac{e^{\alpha r} + q e^{-\alpha r}}{2},
\end{aligned} \tag{2}$$

On the other hand, empirical potential functions for diatomic molecules satisfy the following Varchni's conditions [28]:

$$\left. \frac{dU(r)}{dr} \right|_{r=r_e} = 0, \tag{3}$$

$$U(\infty) - U(r_e) = D_e, \tag{4}$$

$$\left. \frac{d^2U(r)}{dr^2} \right|_{r=r_e} = K_e \equiv (2\pi c)^2 \mu \omega_e^2, \tag{5}$$

where D_e is the dissociation energy, r_e is the equilibrium bond length, c is the speed of light, μ is the reduced mass, and ω_e is the equilibrium harmonic oscillator vibrational frequency.

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Using Varshni's conditions (3) and (4), we can rewrite the potential (1) in the following form:

$$U(r) = D_e \left[1 - \frac{e^{2\alpha r_e} + q}{e^{2\alpha r} + q} \right]^2. \tag{6}$$

This improved Tietz potential has also been obtained for diatomic molecules in [29]. The analytical solutions of the Schrödinger equation with this potential have been investigated [30, 31].

Furthermore, applying Varshni's condition (5) gives:

$$q = -\left(1 - \frac{2\alpha}{\beta}\right) e^{2\alpha r_e}, \tag{7}$$

$$= - \eta e^{2\alpha r_e}, \tag{8}$$

with $\beta = \sqrt{\frac{K_e}{2D_e}}$ and $\eta = \left(1 - \frac{2\alpha}{\beta}\right)$.

On the other hand, the Tietz-Hua oscillator potential [27] is given by:

$$U(r) = D_e \left[\frac{1 - e^{-b_h(r - r_e)}}{1 - c_h e^{-b_h(r - r_e)}} \right]^2 ; \tag{9}$$

where c_h is an optimization parameter and $b_h = \beta(1 - c_h)$. This potential is equivalent to the deformed Schiöberg potential (6) where $\eta = c_h$ and $2\alpha = b_h$ as shown in [21]. In next Section, we will take advantage of this equivalence when solving the potential (6) with the Feynman path integral technique by using the spectroscopic parameters of the diatomic molecules given in Table 1.

3. Solving the Schiöberg-type potential with the path integral method

The basic idea for solving the studied potential with the path integral method is to find an appropriate space-time transformation to reformulate the initial problem in terms of a well-known and already solved problem. Actually, many unknown path integrals have been solved by using their relation to known ones. This method has been discussed in detail in other papers (See references [24, 25, 26]). We present here a brief summary of the essential steps involved.

Let's consider a spherically symmetric effective potential U_{eff} defined by the following:

$$U_{eff}(r_j, \ell) = U(r_j) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}. \tag{10}$$

The propagator for a particle of mass μ in the potential U_{eff} can be developed into a sum of partial waves of the form:

$$k(r^{"}, t^{"}; r^{'}, t^{'}) =$$
$$\frac{1}{4\pi r^{''} r^{'}} \sum_{\ell=0}^{\infty} (2\ell + 1) K_\ell(r^{"}, t^{"}; r^{'}, t^{'}) P_\ell(\cos\theta), \tag{11}$$

where $P_\ell(\cos\theta)$ is the Legendre polynomial and the partial propagator K_ℓ is defined by

$$K_\ell(r^{"}, t^{"}; r^{'}, t^{'}) =$$
$$\lim_{N \to \infty} \int \prod_{j=1}^{N} \exp\left[\frac{i}{\hbar} S_j\right] \prod_{j=1}^{N} \left[\frac{\mu}{2\pi i \hbar \varepsilon}\right]^{\frac{1}{2}} \prod_{j=1}^{N-1} dr_j, \tag{12}$$

with $S_j = \frac{\mu}{2\varepsilon}(\Delta r_j)^2 - \varepsilon U_{eff}(r_j, \ell)$, $\Delta r_j = r_j - r_{j-1}$, $\varepsilon = t_j - t_{j-1}$, $t^{'} = t_0$ and $t'' = t_N$.

This path integral (12) is not solvable for nonzero angular momentum states ($\ell \neq 0$). To overcome this difficulty, we use an approximation for $\frac{1}{r^2}$ centrifugal, given by

$$\frac{r_e^2}{r^2} = C_0 + \frac{C_1}{(e^{2\alpha r} + q)} + \frac{C_2}{(e^{2\alpha r} + q)^2}. \tag{13}$$

The constants C_i can be obtained using a factorization recipe as done in [32, 33]:

$$C_1 = 1 - \left(\frac{1-\eta}{u}\right)^2 \left[\frac{4u}{1-\eta} - (3+u)\right], \tag{14}$$

$$C_2 = 2e^u (1-\eta) \left[3\left(\frac{1-\eta}{u}\right) - (3+u)\left(\frac{1-\eta}{u}\right)^2\right],$$

$$C_2 = \frac{e^{2u}}{u^2}(1-\eta)^4 \left[(3+u) - \frac{2u}{1-\eta}\right].$$

From Table 1, we note that η can take positive or negative values and so is $q = -\eta e^{2\alpha r_e}$. Consequently, the effective potential given in (10) can be put in the following form:

$$U_{eff}(r_j, \ell) = \widetilde{P}_1 + \frac{\widetilde{P}_2}{(e^{2\alpha r_j} + q)} + \frac{\widetilde{P}_3}{(e^{2\alpha r_j} + q)^2}, \tag{15}$$

with

$$\gamma = \frac{\ell(\ell+1)\hbar^2}{2\mu r_e^2}, b = 2\alpha,$$

$$P_1 = D_e, \ P_2 = -2D_e \left(e^{2\alpha r_e} + q\right),$$

$$P_3 = D_e \left(e^{2\alpha r_e} + q\right)^2,$$

$$\widetilde{P}_1 = P_1 + \gamma C_1, \ \widetilde{P}_2 = P_2 + \gamma C_2, \ \widetilde{P}_3 = P_3 + \gamma C_3.$$

Depending on the sign of η, we will consider two cases in the following. We will show that these cases correspond to the deformed Manning-Rosen and the deformed Rosen-Morse potentials. Such a discussion has also been made previously for the particular case of the standard Manning-Rosen and Rosen-Morse potentials in [34].

3.1. Case $\eta < 0$ $(q > 0)$

The potential (15) can be written as

$$U_{eff}(r_j, \ell) = A \tanh_q(\alpha r_j) - \frac{B(\ell)}{\cosh_q^2(\alpha r_j)} + C(\ell), \tag{16}$$

Molecule	η	$\mu/10^{-23}(g)$	$\alpha(\mathring{A}^{-1})$	$r_e(\mathring{A})$	$D_e(cm^{-1})$
$NO(X^2\Pi_r)$	0.013727	1.249	1.357795	1.151	53341
$O_2(X^3\Sigma_g^-)$	0.027262	1.377	1.295515	1.207	42041
$O_2^+(X^2\Pi_g)$	-0.019445	1.377	1.434935	1.116	54688
$N_2(X^1\Sigma_g^+)$	-0.032325	1.171	1.392925	1.097	79885
$H_2(X^1\Sigma_g^+)$	0.170066	0.084	0.80945	0.741	38318
$HF(X^1\Sigma^+)$	0.127772	0.160	0.971035	0.917	49382

Table 1. Spectroscopic molecular parameters for diatomic molecules.

where

$$A = -\frac{\widetilde{P}_2}{2q} - \frac{\widetilde{P}_3}{2q^2}, B(\ell) = \frac{\widetilde{P}_3}{4q}, \quad C(\ell) = \widetilde{P}_1 + \frac{\widetilde{P}_2}{2q} + \frac{\widetilde{P}_3}{2q^2}. \quad (17)$$

Using the translation $y = r_j - \frac{1}{\alpha}\ln\sqrt{q}$, we can easily find the non-deformed potential:

$$U_{eff}(r_j,\ell) = A\tanh(\alpha y) - \frac{B'(\ell)}{\cosh^2(\alpha y)} + C(\ell), \quad (18)$$

where

$$A = -\frac{\widetilde{P}_2}{2q} - \frac{\widetilde{P}_3}{2q^2}, B'(\ell) = \frac{\widetilde{P}_3}{4q^2}, \quad C(\ell) = \widetilde{P}_1 + \frac{\widetilde{P}_2}{2q} + \frac{\widetilde{P}_3}{2q^2}. \quad (19)$$

The effective potential given by (18) is solved in [26] by the Duru-Kleinert method, based on the nonlinear space-time transformation

$$\begin{cases} y = f(z) \\ dt = [f'(z)]^2 d\mathfrak{s}, \end{cases} \quad (20)$$

where $(z,\mathfrak{s})$ are the new space-time coordinates and

$$f(z) = \frac{1}{\alpha}\text{arctanh}\left[2\tanh^2 z - 1\right].$$

Therefore, we can write the propagator associated to the potential (18) in terms of the modified Pöschl-Teller one which is solvable and allows us to compute the following energy spectrum [26]:

$$E_{n,\ell}^{DSch} = -\frac{\hbar^2\alpha^2(s-2n-1)^2}{8\mu} - \frac{2\mu A^2}{\hbar^2\alpha^2(s-2n-1)^2} + C(\ell), \quad (21)$$

with

$$s = \sqrt{1 + \frac{8\mu B'(\ell)}{\hbar^2\alpha^2}}. \quad (22)$$

3.2. Case $\eta > 0$ ($q < 0$)

In terms of hyperbolic functions, the effective potential (15) takes the form

$$\begin{aligned} U_{eff}(r_j,\ell) &= A\coth_q(\alpha r_j) - \frac{B(\ell)}{\sinh_q^2(\alpha r_j)} + C(\ell), \\ &= A\coth(\alpha y) - \frac{B'(\ell)}{\sinh^2(\alpha y)} + C(\ell), \quad (23) \end{aligned}$$

where $y = r_j - \frac{1}{\alpha}\ln\sqrt{-q}$. This potential is similar to the Manning-Rosen one. To solve it, we use the following transformation, as done in [24, 25]:

$$y = \frac{1}{\alpha}\text{arccoth}\left[2\coth^2 z - 1\right]. \quad (24)$$

This leads us to following spectrum

$$E_{n,\ell}^{DSch} = -\frac{\hbar^2\alpha^2(s+2n+1)^2}{8\mu} - \frac{2\mu A^2}{\hbar^2\alpha^2(s+2n+1)^2} + C(\ell). \quad (25)$$

Results (25) and (30) can be combined into one expression

$$E_{n,\ell}^{DSch} = -\frac{\hbar^2\alpha^2(s\pm 2n\pm 1)^2}{8\mu} - \frac{2\mu A^2}{\hbar^2\alpha^2(s\pm 2n\pm 1)^2} + C(\ell). \quad (26)$$

The positive and the negative signs ($\pm$) in (26) correspond to negative and positive values of q respectively.

4. Numerical results and discussions

We show on Figure 1 the variation of the four parameter potential (6). Clearly, the depth of the potential remains constant when the parameter q increases from -1 to 1 (for instance).

We evaluated the accuracy of the energy levels expression (26) for different diatomic molecules: $H_2(X^1\Sigma_g^+)$, $HF(X^1\Sigma^+)$, $N_2(X^1\Sigma_g^+)$, $NO(X^2\Pi_r)$, $O_2(X^3\Sigma_g^-)$ and $O_2^+(X^2\Pi_g)$. We took here molecules with positive and negative values of q. We compared our results to those obtained with state-of-the-art techniques: the numerical method [27] (reference method providing a ground truth), and the supersymmetric quantization (SSQ) (with the same approximation of the barrier) [21]. Results are reported in Table 2, 3, and 4.

Surprisingly, our results are almost identical to those calculated by SSQ in most cases. Indeed, although they are fundamentally different, the two methods use the same approximation of the centrifugal term. In most of the other cases, our technique improves on the SSQ results. This is the case for instance, for the $O_2(X^3\Sigma_g^-)$ molecule ($n = 0, 3, 5$ and $\ell = 10, 15$), for the $O_2^+(X^2\Pi_g)$ ($\ell = 10$ and $n = 1, 3, 5$; $\ell = 15, 20$), and for the molecules $H_2(X^1\Sigma_g^+)$ and $HF(X^1\Sigma^+)$.
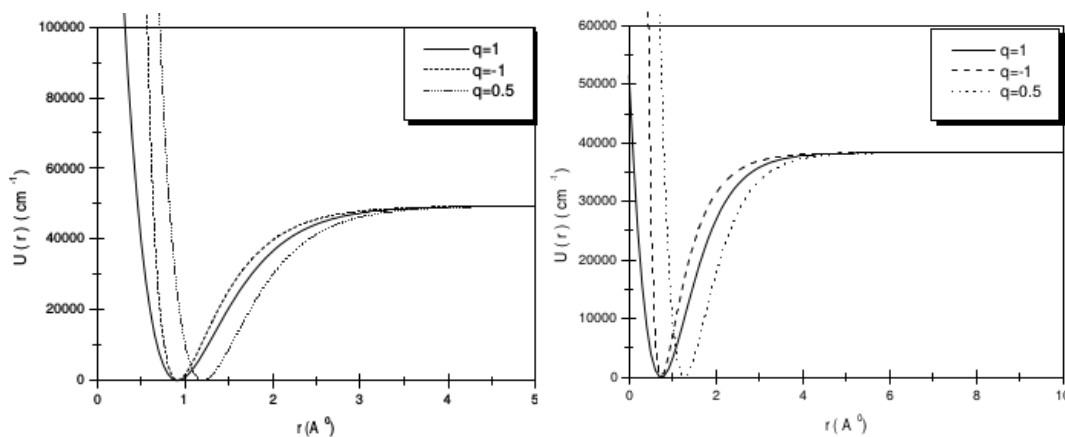
Fig. 1. Variation of the Schiöberg-type potential given in Equation (6) as a function of r for the HF (left) and H_2 (right) diatomic molecule with three different values of q.

5. Conclusion

In this work, we presented and improved expression for the $q-$deformed Schiöberg potential energy function using Feynman path integral method and the equivalence between the studied potential and the Tietz-Hua oscillator potential [21]. We applied this method to calculate the spectrum associated to six diatomic molecules $H_2\left(X^1\Sigma_g^+\right)$, $HF\left(X^1\Sigma^+\right)$, $N_2\left(X^1\Sigma_g^+\right)$, $NO\left(X^2\Pi_r\right)$, $O_2\left(X^3\Sigma_g^-\right)$ and $O_2^+\left(X^2\Pi_g\right)$. Taking the experimental values for the spectroscopic parameters (D_e, r_e, η and α) as inputs, we calculated the numerical values of the energies associated to different n and ℓ. The obtained eigenvalues are in very good agreement with those given by the supersymmetric and the numerical method which proves the efficiency of our method in solving this type of potentials. In the future, we plan to apply this method to solve the Dirac and the Klein-Gorden equations for more general exponential-type potentials.

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Table 2. Ro-vibrational energies $E_{n,l}(cm^{-1})$ $(1\,cm^{-1} = 1.239841930 \times 10^{-4} eV)$ for two diatomic molecules $NO(X^2\Pi_r)$ and $O_2(X^3\Sigma_g^-)$ with $n = 0, 3, 5$ and different value of l.

		$NO(X^2\Pi_r)$			$O_2(X^3\Sigma_g^-)$		
n	l	GPS[27]	SSQ [21]	Our results	GPS[27]	SSQ [21]	Our results
0	0	947.759	947.756	947.757	774.984	775.089	775.090
	1	951.123	951.121	951.120	777.848	777.863	777.860
	2	957.849	957.847	957.847	783.394	783.410	783.411
	3		967.937	967.937		791.731	791.734
	4		981.390	981.390		802.823	802.823
	5		998.205	998.204		816.688	816.682
	10	1132.686	1132.686	1132.686	927.562	927.578	927.574
	15	1351.069	1351.072	1351.072	1107.634	1107.654	1107.648
	20	1653.146	1653.153	1653.153	1356.714	1356.739	1356.744
3	0	6453.267	6453.239	6453.240	5269.581	5269.672	5269.673
	1	6456.510	6456.484	6456.483	5272.250	5272.343	5272.339
	2	6462.995	6462.971	6462.972	5277.588	5277.684	5277.684
	3		6472.703	6472.702		5285.694	5285.697
	4		6485.677	6485.677		5296.374	5296.373
	5		6501.894	6501.894		5309.722	5309.715
	10	6631.552	6631.592	6631.593	5416.325	5416.479	5416.474
	15	6842.080	6842.207	6842.206	5589.607	5589.837	5589.828
	20	7133.275	7133.526	7133.525	5829.279	5829.619	5829.623
5	0	9951.736	9951.693	9951.693	8118.378	8118.516	8118.516
	1	9954.898	9954.857	9954.858	8120.977	8121.118	8121.113
	2	9961.220	9961.188	9961.187	8126.175	8126.321	8126.323
	3		9970.679	9970.679		8134.126	8134.127
	4		9983.335	9983.335		8144.530	8144.529
	5		9999.155	9999.154		8157.535	8157.530
	10	10125.542	10125.669	10125.670	8261.257	8261.546	8261.543
	15	10330.775	10331.112	10331.112	8429.966	8430.441	8430.433
	20	10614.632	10615.269	10615.269	8663.303	8664.046	8664.049

Table 3. Ro-vibrational energies $E_{n,l}(cm^{-1})$ $(1\,cm^{-1} = 1.239841930 \times 10^{-4}eV)$ for two diatomic molecules $O_2^+(X^2\Pi_g)$ and $N_2(X^1\Sigma_g^+)$ with $n = 0,3,5$ and different value of l.

		$O_2^+(X^2\Pi_g)$			$N_2(X^1\Sigma_g^+)$		
n	l	GPS[27]	SSQ[21]	Our results	GPS[27]	SSQ [21]	Our results
0	0	934.601	934.614	934.612	1174.916	1174.927	1174.927
	1	937.848	937.862	937.860	1178.870	1178.882	1178.879
	2	944.341	944.353	944.354	1186.778	1186.789	1186.788
	3		954.094	954.095		1198.651	1198.649
	4		967.079	967.072		1214.466	1214.465
	5		983.310	983.306		1234.234	1234.240
	10	1113.112	1113.127	1113.136	1392.325	1392.338	1392.337
	15	1323.924	1323.940	1323.932	1649.087	1649.103	1649.107
	20	1615.541	1615.563	1615.544	2004.288	2004.306	2004.305
3	0	6376.545	6376.615	6376.612	8047.8758	8047.9316	8047.9313
	1	6379.684	6379.756	6379.755	8051.7163	8051.7736	8051.7718
	2	6385.962	6386.035	6386.034	8059.3972	8059.4558	8059.4546
	3		6395.455	6395.456		8070.9804	8070.9783
	4		6408.015	6408.008		8086.3444	8086.3428
	5		6423.713	6423.708		8105.5492	8105.5556
	10	6549.135	6549.270	6549.277	8259.0350	8259.1477	8259.1462
	15	6752.948	6753.159	6753.151	8508.4072	8508.5904	8508.5949
	20	7034.867	7035.194	7035.186	8853.3707	8853.6563	8853.6550
5	0	9845.984	9846.089	9846.089	12460.466	12460.549	12460.549
	1	9849.051	9849.159	9849.158	12464.229	12464.316	12464.313
	2	9855.183	9855.296	9855.294	12471.756	12471.847	12471.845
	3		9864.503	9864.502		12483.146	12483.143
	4		9876.778	9876.771		12498.208	12498.206
	5		9892.120	9892.117		12517.037	12517.042
	10	10014.566	10014.830	10014.839	12667.396	12667.620	12667.618
	15	10213.639	10214.091	10214.084	12911.769	12912.164	12912.167
	20	10488.989	10489.719	10489.708	13249.806	13250.446	13250.444

Table 4. Ro-vibrational energies $E_{n,l}(cm^{-1})$ ($1\,cm^{-1} = 1.239841930 \times 10^{-4}eV$) for two diatomic molecules $H_2(X^1\Sigma_g^+)$ and $HF(X^1\Sigma^+)$ with $n = 0, 3, 5$ and different value of l.

		$H_2(X^1\Sigma_g^+)$			$HF(X^1\Sigma^+)$		
n	l	GPS[27]	SSQ[21]	Our results	GPS[27]	SSQ [21]	Our results
0	0	2171.618	2171.661	2171.660	2047.581	2047.549	2047.548
	1	2289.372	2289.430	2289.427	2088.368	2088.338	2088.338
	2	2523.795	2523.908	2523.907	2169.893	2169.866	2169.865
	3		2873.012	2873.012		2292.033	2292.033
	4		3333.687	3333.686		2454.691	2454.690
	5		3902.003	3902.002		2657.640	2657.640
	10		8173.796	8173.795		4266.461	4266.460
	15	14184.547	14257.421	14257.418	6824.964	6825.606	6825.605
	20	21121.346	21406.290	21406.287	10257.292	10259.247	10259.246
3	0	13641.123	13641.356	13641.357	13298.712	13298.514	13298.513
	1	13738.726	13740.204	13740.202	13334.713	13334.578	13334.577
	2	13932.924	13937.042	13937.041	13406.668	13406.661	13406.659
	3		14230.181	14230.179		13514.670	13514.669
	4		14617.148	14617.144		13658.467	13658.465
	5		15094.757	15094.756		13837.868	13837.867
	10		18693.126	18693.125		15259.392	15259.390
	15		23846.083	23846.079		17518.249	17518.247
	20		29951.340	29951.338		20544.186	20544.184
5	0	19915.723	19916.031	19916.031	19860.703	19860.423	19860.421
	1	20000.399	20003.596	20003.592	19893.600	19893.479	19893.478
	2	20168.807	20177.985	20177.984	19959.350	19959.547	19959.545
	3		20437.737	20437.735		20058.539	20058.538
	4		20780.713	20780.708		20190.325	20190.323
	5		21204.160	21204.157		20354.730	20354.728
	10		24399.460	24399.458		21656.962	21656.960
	15		28992.500	28992.498		23724.509	23724.507
	20		34465.676	34465.674		26490.600	26490.599