A study of confined quantum systems using the Woods-Saxon potential

A study of confined quantum systems using the Woods–Saxon potential

L S Costa†§, F V Prudente†, P H Acioli†, J J Soares Neto† and
J D M Vianna†‡

† Núcleo de Física Atômica, Molecular e Fluidos, Instituto de Física, Universidade de Brasília,
CP 04455, 70910-900 Brasília DF, Brazil
‡ Instituto de Física, Universidade Federal da Bahia, 40210-340 Salvador BA, Brazil

E-mail: `luis@fis.unb.br` (L S Costa)

Abstract. We propose the Woods–Saxon (WS) potential to simulate spatial confinement. The great advantage of our methodology is that it enables the study of a wide range of systems and confinement regimes by varying two parameters in the model potential. To test the methodology we have studied the confined harmonic oscillator in two different regimes: when the confinement potential exhibits a sudden jump; and when the confinement is described by a smooth function. We have also applied the present procedure to a realistic problem, a confined quantum dot-atom. The numerical calculation is performed with the equally spaced discrete variable representation (DVR). Our results are in close agreement with those available in the literature, and we believe our method to be a good alternative for studying confined quantum systems.

1. Introduction

Confined systems have been studied extensively over the last few years (see [1] and references therein). Interest has increased with the evolution of experimental techniques used in mesoscopic-scale semiconductors structures [2–4].

The study of confined systems is important in catalysis when adsorption phenomena are investigated [5]; in reactions of atoms and molecules inside cavities such as zeolite molecular sieves [6], fullerenes [7, 8] or solvent environments [9], for instance. Moreover, one can study confined phonons [10], polaritons and plasmons [11], gas of bosons [12] and electrons in a quantum dot [13–15].

The influence of spatial confinement on the energy spectra of physical systems is one of the most interesting properties to be investigated in this phenomenon. The usual effects that occur are the increase of the energy values and the degeneracy breaking when the confinement radius decreases [16]. Traditionally, the spatial confinement can be modelled by the imposition of constraint conditions on the wavefunctions [17–22] on the borders of the spatial region, by substitution of the physical potential by a model potential [23] or by introduction of a confinement potential [24–26]. In the third case, the usual additional potential is

$$V(r) = \begin{cases} \infty \text{ or } V_0 = \text{constant} & r \geqslant R \\ 0 & r < R \end{cases} \tag{1}$$

where R defines the region where the system is confined.

§ Author to whom correspondence should be addressed.

In the first and the third cases, the confinement is imposed drastically. Within the confined region, the system is governed by its 'free' physical potential. For many quantum systems these confinement models present problems since the boxing effects are not completely solved [23]. The use of a model potential substituting the physical potential is an attempt to solve this problem. However, in this case, it is necessary to propose one model potential for each confined system to be studied. Consequently, one does not have a general theory.

In this paper, to overcome these difficulties, a novel procedure to study the confinement effects is proposed: (a) we introduce, in the 'free' Hamiltonian, an additional potential that acts over the whole space to simulate the confinement, and (b) we employ a numerical variational method based on wavefunction expansion to compute the eigenenergies of the confined system.

We utilize, as additional potential, the Woods–Saxon (WS) potential function [27]. The WS potential is a continuous function that has two adjustable parameters. These parameters, as we will show, allow one to treat different systems and to simulate smooth model potentials and infinite or finite constant barriers with the same efficiency. The WS potential was used as the optical potential in nuclear reactions almost half a century ago [28]. Recently, the WS potential has been used in molecular physics as an absorbing potential to study, for example, photodissociation [29], chemical reaction [30] and laser-induced processes [31]. Although the WS potential is not a new model potential, its use to simulate the confinement barrier appears to be novel.

As a variational method based on the wavefunction expansion in terms of basis functions we employ the discrete variable representation (DVR) method [29, 32–34]. Such a procedure presents two important qualities: first, this method permits one to calculate various eigenenergies in the same calculation, while traditional procedures calculate a single energy value. Secondly, it is already very well established for the study of non-confined systems and its use can be an effective contribution to analysing confined quantum systems.

To show the efficiency of our method we consider two systems. Initially we study the one-dimensional harmonic oscillator (HO-1D) because it is one of the most extensively used systems for testing new methodologies in quantum mechanics [35]. In fact , in the literature there are several papers on bounded harmonic oscillators [10, 17, 23, 36–41]. We studied the HO-1D in two extreme cases: when the barrier has an abrupt behaviour as in equation (1) and when the barrier is described by a smooth function as in the model potential proposed by Zicovich *et al* [23]. Finally, we apply our method to a real problem: the study of confined electrons in a quantum dot-atom [13–15]. In particular, we calculate the ground state energy of an impurity located in the centre of a parabolic quantum dot.

This paper is organized as follows. In section 2 we show the methodology we use throughout the paper; section 3 is devoted to applications; and in the last section we summarize and present our concluding remarks.

2. Methodology

2.1. The confinement model
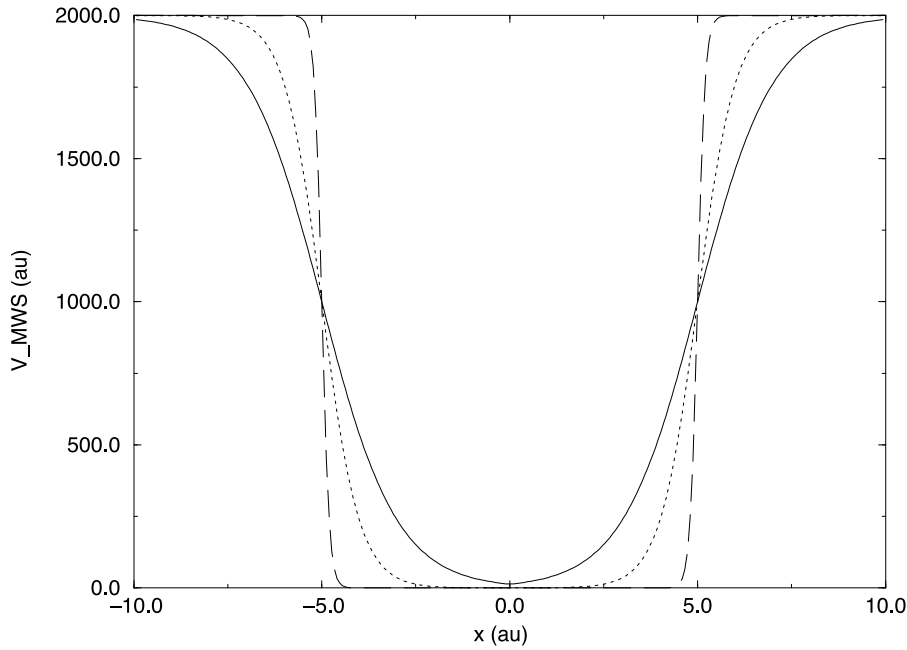
In our procedure, we propose the WS potential to simulate the spatial confinement. For this, we add the WS potential

$$V_{WS}(x; R) = \frac{2\lambda}{1 + \exp[(R - x)/\eta]} \tag{2}$$

into the 'free' Hamiltonian of the quantum system. In equation (2) R defines the confinement barrier position, λ controls the barrier height and η controls its slope. These parameters

Figure 1. General form of modified Woods–Saxon potential.

guarantee the flexibility of the present methodology treating a great variety of confined systems. We notice that the WS potential assumes the value λ when $x = R$.

We utilize expression (2) to introduce the confinement barrier into problems that have spherical symmetry (i.e. the x range is from 0 to ∞) and, for a system with two symmetric spatial confinement barriers ($-R < x < R$), we modify the usual WS potential and obtain:

$$V_{\text{MWS}}(x; R) = \begin{cases} \dfrac{2\lambda}{1 + \exp[(R + x)/\eta]} & x < 0 \\[2ex] \dfrac{2\lambda}{1 + \exp[(R - x)/\eta]} & x > 0 \end{cases} \tag{3}$$

where R, η and λ are defined as in equation (2). We call it the modified Woods–Saxon potential (V_{MWS}). Figure 1 shows the V_{MWS} for different values of η. We emphasize that the barrier inclination increases as the η parameter decreases.

The most important advantage of our proposal is that the WS potential is able to represent several confinement models simply by adjusting the parameters η and λ, while the current procedures use a confinement potential for each system. All we need is to obtain the parameters η and λ which describe well the physical system in question. To optimize the parameters η and λ we have minimized the mean-square deviation between the computed eigenvalues and the expected (experimental or theoretical) results. For the minimization procedure we have used Powell's direction set method [42].

2.2. Equally spaced discrete variable representation

In this work we use a variational method based on wavefunction expansion, namely DVR, to solve the Schrödinger equation of confined systems.

The DVR method expands the wavefunction using a set of basis functions $\{f_i(x)\}$ with the following property:

$$f_i(x_j) = \delta_{ij} \tag{4}$$

where x_j are the points of a Gaussian quadrature rule. Thus, the elements of the potential energy matrix are given by

$$V_{ij} = V(x_i)\,\delta_{ij}. \tag{5}$$

The kinetic energy matrix elements are calculated analytically [32]. The grid of the equally spaced DVR is

$$x_i = a + \frac{(b-a)\,i}{N} \qquad i = 1, \ldots, N-1 \tag{6}$$

and the associated functions used to build the basis functions $\{f_j\}$ for this grid are

$$g_j(x) = \left(\frac{2}{b-a}\right)^{1/2} \sin\left[\frac{j\pi(x-a)}{b-a}\right] \qquad j = 1, \ldots, N-1. \tag{7}$$

The elements of the kinetic energy matrix in the DVR are then,

$$T_{ii'} = \langle f_i|\hat{T}|f_{i'}\rangle = \frac{-\hbar^2}{2m}\Delta x \sum_{n=1}^{N-1}\sum_{m=1}^{N-1} g_n^*(x_i)\,g_m(x_{i'}) \int g_n^*(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2} g_m(x)\,\mathrm{d}x \tag{8}$$

with a grid spacing of

$$\Delta x = \frac{(b-a)}{N}. \tag{9}$$

We substitute the associated functions in the expression above and obtain the elements of the kinetic energy matrix [32],

$$T_{ii'} = \frac{\hbar^2}{2m}\frac{(-1)^{i-i'}}{(b-a)^2}\frac{\pi^2}{2}\left\{\frac{1}{\sin^2\left[\pi(i-i')/2N\right]} - \frac{1}{\sin^2\left[\pi(i+i')/2N\right]}\right\} \qquad i \neq i' \tag{10}$$

and

$$T_{ii'} = \frac{\hbar^2}{2m}\frac{1}{(b-a)^2}\frac{\pi^2}{2}\left\{\frac{(2N^2+1)}{3} - \frac{1}{\sin^2\left[\pi(i)/N\right]}\right\} \qquad i = i'. \tag{11}$$

We note that these expressions depend only on the grid points; so, they are a general expression for all one-dimensional systems. However, this procedure is extended easily to two- and three-dimensional systems [43, 44].

3. Confined harmonic oscillator results

The confined HO-1D has been used in the literature to explain some experimentally observed deviations from the results predicted by calculations based on the free harmonic oscillator model. In particular, one can cite the emission spectra of the luminescence centres in crystals [10] and the infrared stretching transition of the porphine [23]. Recently, it has been utilized to investigate the confinement effect in the vibrational energies of point defects, impurities or luminescence centres in solids [1, 17, 23].

To study the confined HO-1D with our model, we start from the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \right] \Psi(x) = E\Psi(x) \tag{12}$$

with $V(x)$ given by

$$V(x) = \tfrac{1}{2}kx^2 + V_{\text{MWS}}(x; R) \tag{13}$$

where R is the confinement radius and $V_{\text{MWS}}(x; R)$ is the modified Woods–Saxon potential, given by equation (3). In order, we optimize the parameters η and λ according to the spatial confinement required. This technique is employed to find numerical results in two different cases.

3.1. Confined HO-1D with Zicovich-Wilson model potential

In order to simulate (with equation (13)) the Zicovich-Wilson *et al* [23] confined potential given by

$$V(x) = \frac{k}{2}\left(\frac{\tan\alpha x}{\alpha}\right)^2 \qquad \alpha = \frac{\pi}{2R} \tag{14}$$

we have utilized our optimization process to obtain the parameters η and λ shown in table 2. Then, the eigenenergies have been calculated using 300 equally spaced points between -5.0

Table 1. Energy eigenvalues for confined HO-1D using our method (V_{MWS}) and the Zicovich-Wilson model potential (ZWPJ) ($\hbar = 1, m = 1, k = 1$).

State	R	V_{MWS}	ZWPJ [23]
0	0.5	4.979 35	4.984 63
0	1.0	1.395 37	1.410 56
0	2.0	0.673 37	0.677 45
0	3.0	0.580 08	0.573 21
0	4.0	0.548 41	0.540 04
1	0.5	19.881 22	19.888 35
1	1.0	5.445 07	5.464 95
1	2.0	2.333 41	2.340 79
1	3.0	1.855 33	1.856 72
1	4.0	1.696 00	1.697 22
2	0.5	44.668 56	44.661 01
2	1.0	12.008 43	11.985 83
2	2.0	4.631 98	4.620 97
2	3.0	3.402 11	3.414 38
2	4.0	2.989 25	3.008 61
3	0.5	79.322 91	79.302 61
3	1.0	21.030 05	20.973 07
3	2.0	7.545 99	7.518 00
3	3.0	5.241 03	5.246 20
3	4.0	4.457 43	4.474 22
4	0.5	123.802 03	123.813 13
4	1.0	32.400 33	32.426 60
4	2.0	11.016 35	11.031 89
4	3.0	7.361 411	7.352 18
4	4.0	6.107 98	6.094 04

Table 2. Optimized Woods–Saxon parameters for table 1.

R	$1/\eta$	2λ
0.5	125.389 192	4057.702 893
1.0	23.103 249	247.319 375
2.0	5.786 116	82.141 693
3.0	3.501 985	123.827 642
4.0	2.808 746	318.422 328

Table 3. Energy eigenvalues for confined HO-1D with constant infinite barrier using our method (V_{MWS}), analytical quantum procedure (CF) and modified WKB (AM) ($\hbar = 1$, $m = 1$, $k = \frac{1}{4}$).

State	$R\sqrt{2}$	CF [38]	AM [39]	V_{MWS}
0	0.5	9.87	9.88	9.871 69
0	1.0	2.48	2.48	2.476 45
0	2.0	0.65	0.67	0.649 78
0	3.0	0.34	0.38	0.343 73
0	4.0	0.27	0.30	0.268 78
1	0.5	39.48	39.55	39.479 54
1	1.0	9.89	9.90	9.890 81
1	2.0	2.54	2.54	2.540 07
1	3.0	1.25	1.26	1.249 17
1	4.0	0.88	0.90	0.882 69
2	0.5			88.807 53
2	1.0			22.233 99
2	2.0			5.634 59
2	3.0			4.552 98
2	4.0			1.700 70
3	0.5			157.841 27
3	1.0			39.512 60
3	2.0			9.959 07
3	3.0			7.014 16
3	4.0			2.792 91
4	0.5			246.546 76
4	1.0			61.727 34
4	2.0			15.516 94
4	3.0			10.020 51
4	4.0			4.187 05

and 5.0 au to build the DVR. Table 1 shows our energy eigenvalues for a few confinement radius values ($R = 0.5, 1.0, 2.0, 3.0, 4.0$) along with the exact values. In the calculations we have used $\hbar = 1$, $m = 1$, $k = 1$. Our results are in very good agreement with the results obtained by Zicovich-Wilson *et al*.

3.2. Confined HO-1D with constant infinite barrier

The other system that we have studied is the confined HO-1D with an infinite barrier (equation (1)). In this case, our optimization procedure for the parameters η and λ gives the values shown in table 4. To calculate the eigenenergies we have utilized 300 equally spaced points between -4.0 and 4.0 au to build the DVR. Table 3 shows our energy eigenvalues for five

Table 4. Optimized Woods–Saxon parameters for table 3.

$R\sqrt{2}$	$1/\eta$	2λ
0.5	874.249 724	9 999 999 999.615 74
1.0	2869.938 606	10 000 001.036 3109
2.0	932.295 493	9 999 999 999.999 03
3.0	1143.937 374	10 000 000.416 3662
4.0	1192.643 669	10 000 000 000.000 0

confinement radius values ($R\sqrt{2} = 0.5, 1.0, 2.0, 3.0, 4.0$). The results obtained by Adams and Miller using the modified WKB method [39] and by Consortini and Frieden with an analytical quantum procedure [38] are presented for comparison. In these calculations $\hbar = 1$, $m = 1$, $k = \frac{1}{4}$. One sees that our results are in quite good agreement with the results in the literature.

Concluding this section, we remark that the confined HO-1D using two different potentials is described, in our methodology, by only one potential function, $V_{\mathrm{MWS}}(x)$.

4. Quantum dot-atom results

We have applied our method to a real problem, the study of a quantum dot-atom. We can consider this system as an artificial atom [45] since quantum dots are small conductive regions in a semiconductor that occupy well defined discrete quantum states. Recently, the problem of an impurity in the centre of one parabolic quantum dot was studied by variational methods where the central question was the choice of the trial wavefunction [13, 15]. The Hamiltonian in the effective-mass approximation and using atomic units is [13]

$$H = -\nabla^2 - \frac{2}{r} + \gamma_p^2 r^2 \tag{15}$$

where $\gamma_p = \hbar\omega_p/2Ry$

This problem was solved by Xiao *et al* [15] and by Varshni [13] utilizing the variational method for two different types of trial wavefunctions. Varshni [13] presents numerical results obtained by integration of the Schrödinger equation using Numerov's method and a logarithmic mesh. These values can be considered as exact solutions for the energy and we utilize them to compare with our calculations.

To apply our procedure to a quantum dot-atom, we introduce the WS potential (equation (2)) into the Hamiltonian (15) and obtain

$$H = -\nabla^2 - \frac{2}{r} + \gamma_p^2 r^2 + V_{\mathrm{WS}}(r; R). \tag{16}$$

The eigenenergies are determined by using the optimization of the parameters η and λ, and the DVR method. We have considered various confinement radii and three values of γ_p. Table 5 shows, for all studied values of γ_p, the binding energies (defined by Varshni [13]) and the optimized WS parameters we have obtained. Exact binding energy values are also shown for comparison. One sees that our results reproduce the exact energy with great precision for all values of confinement radius R and γ_p parameter considered. These results together with those obtained in the confined HO-1D study demonstrate the strength of our methodology of combining the WS model potential with the DVR method to study confined quantum systems.

Table 5. Optimized Woods–Saxon parameters and binding energy values for a real problem (an impurity in a parabolic quantum dot) using our method (V_{WS}), and Varshni's exact values (Vars).

R	$1/\eta$	2λ	V_{WS}	Vars [13]	γ_p
1.0	86.754 759	2993.473 288	5.152 486	5.152 486	0.2
1.0	88.340 541	2993.466 669	5.153 915	5.153 915	0.3
1.0	88.342 176	2993.465 715	5.155 917	5.155 917	0.4
1.2	89.709 729	2993.535 879	4.336 610	4.336 610	0.2
1.2	89.711 108	2993.513 964	4.339 140	4.339 140	0.3
1.2	89.713 501	2993.476 543	4.342 682	4.342 682	0.4
1.4	91.105 971	2993.419 025	3.757 820	3.757 820	0.2
1.4	91.110 087	2993.419 026	3.761 925	3.761 925	0.3
1.4	91.114 355	2993.419 027	3.767 670	3.767 670	0.4
1.6	92.476 838	2994.262 002	3.327 101	3.327 101	0.2
1.6	92.476 838	2994.120 259	3.333 348	3.333 348	0.3
1.6	92.486 674	2994.268 769	3.342 090	3.342 090	0.4
1.8	94.179 994	2998.822 361	2.995 187	2.995 187	0.2
1.8	94.188 063	2998.711 200	3.004 240	3.004 240	0.3
1.8	94.122 201	2994.303 584	3.016 904	3.016 904	0.4
2.0	95.675 910	2993.399 842	2.732 638	2.732 638	0.2
2.0	95.696 075	2993.429 949	2.745 262	2.745 262	0.3
2.0	95.722 799	2993.423 707	2.762 897	2.762 897	0.4
2.2	97.365 268	2993.473 005	2.520 791	2.520 791	0.2
2.2	97.397 103	2993.498 118	2.537 836	2.537 836	0.3
2.2	97.451 289	2993.474 996	2.561 606	2.561 606	0.4
2.4	99.223 527	2995.711 209	2.347 243	2.347 243	0.2
2.4	99.236 976	2993.403 450	2.369 645	2.369 645	0.3
2.4	99.370 808	2995.654 161	2.400 794	2.400 794	0.4
2.6	101.119 071	2993.476 605	2.203 432	2.203 432	0.2
2.6	101.217 406	2993.482 475	2.232 194	2.232 194	0.3
2.6	101.413 847	2993.431 075	2.272 008	2.272 008	0.4
2.8	103.232 033	2993.479 555	2.083 266	2.083 266	0.2
2.8	103.441 522	2993.479 134	2.119 434	2.119 434	0.3
2.8	103.792 054	2993.484 525	2.169 170	2.169 170	0.4
3.0	105.602 453	2994.562 167	1.982 281	1.982 281	0.2
3.0	105.993 863	2994.448 853	2.026 906	2.026 906	0.3
3.0	106.701 360	2994.595 237	2.087 713	2.087 713	0.4
4.0	127.355 689	2993.460 078	1.670 637	1.670 637	0.2
4.0	126.181 523	2994.322 813	1.770 142	1.770 142	0.3
4.0	211.185 350	2995.657 302	1.892 868	1.892 868	0.4
5.0	47.274 217	445.112 383 0	1.545 602	1.545 602	0.2
5.0	2451.832 229	268.900 655 1	1.700 058	1.700 058	0.3
5.0	2455.073 658	1.841 043 423	1.861 207	1.861 207	0.4
6.0	393.531 103	19.945 059 25	1.505 747	1.505 747	0.2
6.0	105.814 563	2994.595 237	1.689 308	1.689 316	0.3
6.0	91.105 971	2993.419 025	1.859 172	1.859 181	0.4
7.0	471.792 157	2.362 595 237	1.497 086	1.497 088	0.2
7.0	471.814 563	2.362 595 237	1.688 523	1.688 530	0.3
7.0	472.597 096	2.993 419 025 5	1.859 125	1.859 134	0.3

5. Summary of results and conclusion

We have proposed a novel procedure to study the confinement effects in quantum systems, i.e. the use of the WS potential function to simulate the spatial confinement and the use of variational methods to calculate the energy spectra. In particular, we have used the equally spaced discrete variable representation method (DVR). We have applied the present methodology to study the confinement effects in two quantum systems: the one-dimensional harmonic oscillator in two different confinement regimes (the model potential proposed by Zicovich-Wilson *et al* and the HO-1D confined between infinite rectangular walls) and the parabolic quantum dot-atom in the presence of an impurity. Our results are in close agreement with those available in the literature.

We point out some important aspects of the present results. First, the flexibility of the methodology: using the same functional form of the Hamiltonian, equations (12) and (13), we have studied two different ways of confining the harmonic oscillator, simply by varying the WS parameters. Secondly, the same methodology can be applied to different systems: in this work we have treated the confined HO-1D and a quantum dot-atom with the same procedure, obtaining accurate results in both cases. Thirdly, the efficiency of the methodology: we have obtained both ground and excited states in the same calculation, while the usual methods are restricted to computing only one state. In addition, the present methodology has the important advantage that it can be applied to a variety of quantum systems without the need for new potential models or trial wavefunctions.

We conclude that the WS potential simulates different confinement barriers very well and can be used in the analysis of the energy spectra of confined systems using the same numerical procedure (DVR) utilized in 'free' systems. Consequently, the present procedure can be an effective contribution in the area of confined systems since these numerical techniques are already very well established and can be readily extended to three-dimensional systems. In this context there are several questions to be analysed with the present confinement model: the study of rotational and electronic spectra of diatomic molecules, the study of triatomic molecules and the artificial molecule composed from the connection of two quantum dot-atoms [46], are some examples. Work in these directions is in progress and will be published elsewhere.

References

[1] Jakólski W 1996 *Phys. Rep.* **271** 1
[2] Esaki L and Chang L L 1974 *Phys. Rev. Lett.* **33** 495
[3] Dingle R, Wiegmann W and Henry C H 1974 *Phys. Rev. Lett.* **33** 827
[4] Reed M A, Randall J M, Aggarwal R J, Matyi R J, Moore T M and Wetsel A E 1988 *Phys. Rev. Lett.* **60** 535
[5] Frank K H, Didde R, Sagner H J and Eberhardt W 1989 *Phys. Rev.* B **39** 940
[6] Tang Z K, Nozue Y and Goto T J 1992 *Phys. Soc. Japan* **61** 2943
[7] Kroto H W, Heath J R, O'Brian S C, Curl R F and Smalley R E 1985 *Nature* **318** 162
[8] Lazlo I and Udvardi L 1987 *Chem. Phys. Lett.* **136** 418
[9] Reichardt C 1988 *Solvents and Solvents Effects in Organic Chemistry* (Weinheim: VCH)
[10] Grinberg M, Jaskólski W, Kopke Cz, Plannelles J and Jnowicz M 1994 *Phys. Rev.* B **50** 6504
[11] Gudmundson V and Gerhardts R R 1991 *Phys. Rev.* B **43** 12 098
[12] Gudmundson V and Holthaus M 1995 *Z. Phys.* B **97** 319

[13] Varshni Y P 1998 *Superlattices Microstuct.* **23** 145
[14] Kumar A, Laux S E and Stern F 1990 *Phys. Rev.* B **42** 5166
[15] Xiao Z, Zhu J and He F 1996 *Superlattices Microstruct.* **19** 137
[16] Aquino N 1997 *J. Phys. A: Math. Gen.* **30** 2403
[17] Goodfriend P L 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** 1373
[18] Satpatly S 1983 *Phys. Rev.* B **28** 4585
[19] Kovalenko A F, Sovjak E N and Golovko 1989 *Phys. Stat. Solidi* b **155** 549
[20] Lee-Koo E and Garcia-Castelon R M G 1991 *Phys. Rev.* A **24** 1481
[21] Marin J L and Cruz S A 1991 *Am. J. Phys* **59** 931
[22] Varshni Y P 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** L589
[23] Zicovich-Wilson C, Planelles J H and Jakólski W 1994 *Int. J. Quantum Chem.* **50** 429
[24] Chuu D S, Hsiao C M and Mei W N 1992 *Phys. Rev.* B **46** 3898
[25] Ley-Koo E and Rubinstein 1979 *J. Chem. Phys.* **71** 351
[26] Vawter R 1968 *Phys. Rev.* **174** 749
[27] Woods R D and Saxon D S 1954 *Phys. Rev.* **95** 577
[28] Feshbach H 1958 *Ann. Rev. Nucl. Sci.* **8** 49
[29] Seideman T 1993 *J. Chem. Phys.* **98** 1989
[30] Seideman T and Miller W H 1992 *J. Chem. Phys.* **97** 2499
[31] Leforestier C and Wyatt R E 1983 *J. Chem. Phys.* **78** 2334
[32] Colbert D T and Miller W H 1992 *J. Chem. Phys.* **9** 1982
[33] Muckerman J T 1990 *Chem. Phys. Lett.* **173** 200
[34] Prudente F V, Costa L S and Soares Neto J J 1997 *J. Mol. Struct. (Theochem)* **394** 169
[35] Wehrhahn R F and Cooper L 1992 *J. Math. Phys.* **33** 174
     Fradkin D M 1992 *J. Math. Phys.* **33** 1705
[36] Baijal J S and Singh K K 1955 *Prog. Theor. Phys.* **14** 214
[37] Vawter R 1968 *Phys. Rev.* **174** 749
[38] Consortini A and Frieden B R 1976 *Nuovo Cimento* B **35** 153
[39] Adams J E and Miller W H 1977 *J. Chem. Phys.* **67** 5775
[40] Rotbart F C 1978 *J. Phys. A: Math. Gen.* **11** 2363
[41] Larsen U 1983 *J. Phys. A: Math. Gen.* **16** 2137
[42] Press W H, Flanney B P, Tenkolsky S A and Vetteiling W T 1989 *Numerical Recipes* (Cambridge: Cambridge
     University Press)
[43] Witnell R M and Light J C 1989 *J. Chem. Phys.* **90** 1774
[44] Wei H and Carrington T Jr 1992 *J. Chem. Phys.* **97** 3029
[45] Ashori R 1996 *Nature* **379** 413
[46] Dosterkamp T H, Fujisawa T, van der Wiel W G, Ishibashi K, Hijman R V and Kouwenhoven L P 1998 *Nature*
     395 823