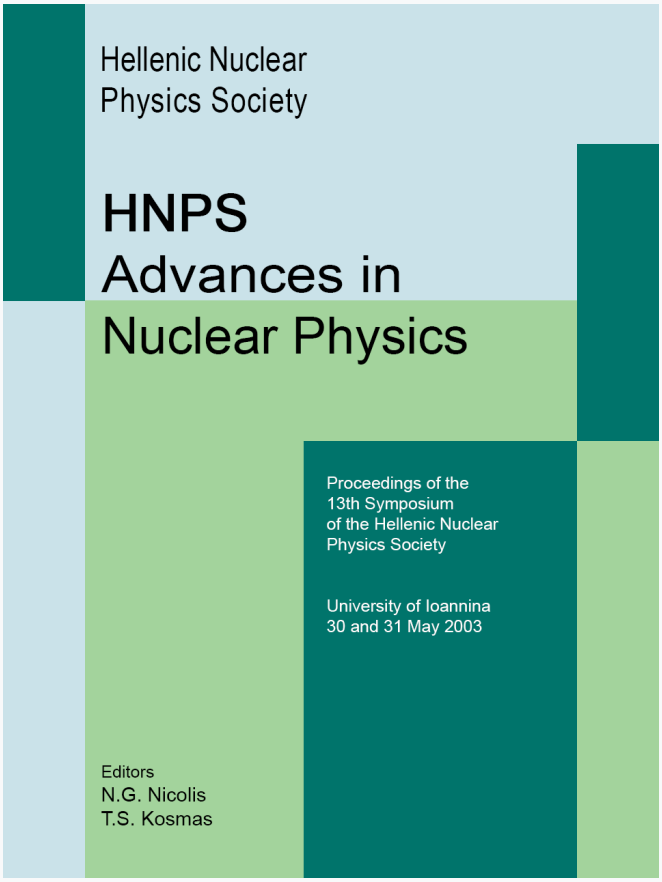
HNPS Advances in Nuclear Physics

Vol 12 (2003)

HNPS2003



The HVT Technique and the "Uncertainty" Relation for Central

M. Grypeos, C. G. Koutroulos, K. J. Oyewumi, Th. Petridou

doi: 10.12681/hnps.3351

HNPS Advances in Nuclear Physics vol. 12, pp. 118-129 (2003)
HNPS2003
doi:10.12681/hnps.3351

THE HVT TECHNIQUE AND THE "UNCERTAINTY" RELATION FOR CENTRAL POTENTIALS

M.E. Grypeos, C.G. Koutroulos, K.J. Oyewumi+, Th. Petridou
Department of Theoretical Physics, Aristotle University of Thessaloniki, Greece

+ Permanent address: Physics Department, University of Ilorin, Nigeria.

The quantum mechanical hypervirial theorems (HVT) technique is used to treat the so-called "uncertainty" relation for quite a wide class of central potential wells, including the (reduced) Poeschl-Teller and the Gaussian one. It is shown that this technique is quite suitable in deriving an approximate analytic expression in the form of a truncated power series expansion for the dimensionless product $P_{nl} \equiv < r^2 >_{nl} < p^2 >_{nl} / \hbar^2$, for every (deeply) bound state of a particle moving non-relativistically in the well, provided that a (dimensionless) parameter s is sufficiently small. Numerical results are also given and discussed.

PACS numbers:02,60-x,03.65.-w,21.80.+a

1. Introduction

The quantum mechanical hypervirial theorems (HVT) technique [1,2] is a very useful technique in dealing with various problems encountered in Physics and Chemistry. Its main advantage is that one can calculate expectation values of interesting quantities, avoiding the use of the wave function and thus achieving considerable simplification. Particular attention was paid in obtaining energy eigenvalues for a particle moving in a potential and a lot of work has been done in this direction for various types of potentials [3].

The case of a general class of even-power series central potentials and in particular those of the form $V(r) = -V_0 f(\frac{r}{R})$ was studied in refs. [4,5]. In that procedure, one obtains in a unified way the general expressions of the (lower) bound state energy eigenvalues and of the expectation values of certain other physical quantities with respect to the eigenstates of the single particle Hamiltonian. Application of these expressions to specific potentials

of the class leads immediately to the corresponding expressions for the particular potential considered. Those expressions are of the form of expansions in powers of a small parameter and the first terms of the expansions are expected to provide a reasonable approximation of the calculated quantities, as long as the parameter is sufficiently small. For potentials of the form $V(r) = -V_0 f(\frac{r}{R})$, the expressions are power-series of the dimensionless parameter $s = (\frac{\hbar^2}{2\mu V_0 R^2})^{1/2}$ and the structure of the first terms of the expansions is fairly simple. The successive terms of each expansion are obtained by means of suitable recurrence relations on the basis of Swenson and Danforth hypervirial relations [6] and the Hellmann-Feynman theorem [7]. See also Killingbeck [2].

In a recent publication [8] another useful application of the HVT technique was considered, namely the study of inequalities of physical interest. Two basic inequalities were studied, relating the lowest energy level spacing ΔE of a particle in its ground state, moving non-relativistically in a central well, with the mean-square radius of its orbit and the expectation value of its kinetic energy, respectively, with the aim of investigating their (approximate) "saturation", that is whether they become equalities approximately (e.g. within a few per cent) [9].

The aim of the present work is to discuss another inequality which is important to Physics. It has been pointed out (see ref. [10] and section 2 of ref.[11]) that for a particle moving non-relativistically in a central potential $V(r)$, the following "uncertainty" relation holds

$$< r^2 >< p^2 > /\hbar^2 \geq \frac{9}{4} \tag{1}$$

It was pointed out that the inequality becomes equality for the ground state of the harmonic oscillator potential (HO). In all other cases the above relation is an inequality and it would be of interest to provide analytic ways in calculating the dimensionless product $P_{nl} \equiv < r^2 >< p^2 > /\hbar^2 \geq \frac{9}{4}$, where the expectation values are calculated with respect to the hamiltonian single particle eigenstates. That would provide the means to investigate to what extent the inequality is saturated, depending on the potential shape considered and on the specific state. We may recall that the usual uncertainty relation for the position and its conjugate momentum: $\Delta\hat{x}\Delta\hat{p} \geq \hbar/2$ and its generalizations has been the subject of detailed investigations since the

publication of Heisenberg's original paper [12] until recently (see e.g. ref.[13] and references therein). We refer in this respect to the very informative review article [14a]. Among the topics of interest has been the analytic calculations of the uncertainty product $(\Delta\hat{x})(\Delta\hat{p})$ for various types of one-dimensional potentials (see e.g. ref.[14b]).

The formalism and the expression for P_{nl} are given in the next section, while in the final one numerical results are given and discussed.

2. The formalism and the expression for the dimensionless product P_{nl}

In this section the s-power series expansions, mentioned in the introduction and which had been derived [4,5] by means of the HVT technique are used.

The wide class of two-parameter potential wells of the general form:

$$V(r) = -V_o f(r/R), \qquad 0 \leq r < \infty \tag{2}$$

is considered and a particle of mass μ is assumed to move (non-relativistically) in a well of this form. In the above expression, $V_o > 0$ is the potential depth, $R > 0$ its "radius" and f $(f(0) = 1)$ the "potential form factor" which determines its shape. The function f is assumed to be an appropriate analytic function of even powers of $x = r/R$ with $d^2 f/dx^2|_{x=0} < 0$. Such potentials behave like an harmonic oscillator potential near the origin and therefore the terminology "oscillator-like" potentials has been used. The results of this work corroborate the suitability in using such a terminology (see section 3). Apart from the above mentioned resemblence, their shape is quite different from that of the harmonic oscillator.

Typical potentials of the class are:

a) The Gaussian potential

$$V_G(r) = -V_o e^{-r^2/R^2}$$

b) The (reduced) Poeschl-Teller (PT) potential

$$V_{PT}(r) = -V_o cosh^{-2}(r/R)$$

but there are many other belonging to the same class.

In order to obtain the dimensionless product P_{nl} it is convenient to use for the energy eigenvalues and the expectation values of the kinetic energies and the mean square radii of the particle orbits the dimensionless expressions of their s-expansions of ref.[5] which are denoted by a tilde on the top of the corresponding symbols. In the pertinent formulae, displayed below, it was found appropriate to rearrange somehow the terms in the coefficients of powers greater than 2, so that there is a more convenient way in factorizing the two sorts of contributions, that is those originating from the quantum numbers nl of the state and those from the numbers d_k, determined by the potential shape, which are related to the derivatives of the potential form factor f:

$$d_k = \frac{1}{(2k)!}\frac{d^{2k}}{dx^{2k}} f(x)|_{x=0} \quad , \qquad k = 0, 1, 2, ..., \qquad d_1 < 0 \tag{3}$$

The above rearrangement of terms in the coefficients of the s-powers will facilitate their use in the following.

We also note that it would be desirable to consider in addition a renormalized hypervirial perturbation theory [2,15] which is a very efficient one and has been used in treating various problems [16,17]. This matter is under investigation and requires further work in order that the method is adjusted to our purposes.

The expression of the expansion for the energy eigenvalues is as follows:

$$\tilde{E}_{nl} = \frac{E_{nl}}{V_0} = \sum_{k=0}^{\infty} e_k s^k \tag{4}$$

where

$$e_0 = -1 \tag{5}$$

$$e_1 = 2a_{nl}(-d_1)^{1/2}, \quad a_{nl} = (2n + l + \frac{3}{2}) \tag{6}$$

$$e_2 = \frac{d_2}{8d_1}(12a_{nl}^2 - 4l(l+1) + 3) \tag{7}$$

$$e_3 = -\frac{a_{nl}(-d_1)^{1/2}}{32d_1^3}$$
$$\{4d_1d_3[20a_{nl}^2 - 12l(l+1) + 25] + d_2^2[-68a_{nl}^2 + 36l(l+1) - 67]\} \tag{8}$$

$$e_4 = \frac{1}{1024d_1^4}\{12d_1d_2d_3[880a_{nl}^4 - 8a_{nl}^2[84l(l+1) - 295] + 3[4l(l+1) - 3]$$
$$[4l(l+1) - 35]] + d_2^3\left[-6000a_{nl}^4 + 24a_{nl}^2[172l(l+1) - 569] - \right.$$
$$[4l(l+1) - 3][44l(l+1) - 513]] + 8d_1^2d_4\left[-560a_{nl}^4 + 40a_{nl}^2[12l(l+1) - 49]\right.$$
$$-3[4l(l+1) - 3][4l(l+1) - 35]]\} \tag{9}$$

For the mean-square radii of the particle orbits we have

$$< \widetilde{r^2} >_{nl} \equiv \frac{< r^2 >_{nl}}{R^2} = \sum_{k=0}^{\infty} r_k s^k \tag{10}$$

where

$$r_0 = 0 \tag{11}$$

$$r_1 = \frac{a_{nl}}{(-d_1)^{1/2}} \tag{12}$$

$$r_2 = \frac{d_2}{8d_1^2}(12a_{nl}^2 - 4l(l+1) + 3) \tag{13}$$

$$r_3 = -\frac{a_{nl}(-d_1)^{1/2}}{64d_1^4}.$$
$$\left\{12d_1d_3(20a_{nl}^2 - 12l(l+1) + 25) + 5d_2^2\left[-68a_{nl}^2 + 36l(l+1) - 67\right]\right\} \tag{14}$$

$$r_4 = -\frac{1}{256d_1^5}\{9d_1d_2d_3[-880a_{nl}^4 + 8a_{nl}^2[84l(l+1) - 295] - 3[4l(l+1) - 3]$$
$$[4l(l+1) - 35]] + d_2^3\left[6000a_{nl}^4 - 24a_{nl}^2[172l(l+1) - 569] + \right.$$

$$[4l(l+1)-3][44l(l+1)-513]] + 4d_1^2 d_4 \Big[560a_{nl}^4 - 40a_{nl}^2[12l(l+1)-49]+ 3[4l(l+1)-3][4l(l+1)-35]]\} \quad (15)$$

Finally, for the expectation value of the kinetic energy operator in the various energy eigenstates we have:

$$< \widetilde{T} >_{nl} \equiv \frac{T_{nl}}{V_0} = \sum_{k=0}^{\infty} t_k s^k \quad (16)$$

where

$$t_k = \frac{k}{2} e_k, \qquad k = 0, 1, 2..... \quad (17)$$

For the product $< r^2 >_{nl} < p^2 >_{nl}$ we may write

$$\begin{aligned} < r^2 >_{nl} < p^2 >_{nl} &= 2\mu V_0 R^2 < \widetilde{r}^2 >_{nl} < \widetilde{T} >_{nl} \\ &= \frac{\hbar^2}{s^2} < \widetilde{r}^2 >_{nl} < \widetilde{T} >_{nl} \\ &= \frac{\hbar^2}{s^2} (\sum_{k=0}^{\infty} r_k s^k)(\sum_{k=0}^{\infty} t_k s^k) \\ &= \frac{\hbar^2}{s^2} (\sum_{k=0}^{\infty} \gamma_k s^k) \end{aligned} \quad (18)$$

where

$$\gamma_k = (\sum_{\rho=0}^{k} r_\rho t_{k-\rho}) \quad (19)$$

The expressions of $\gamma_k, k = 0, 1, 2...$ follow easily from the expressions of r_k and t_k. We find

$$\begin{aligned} &\gamma_0 = \gamma_1 = 0, \quad \gamma_2 = r_1 t_1 = a_{nl}^2, \\ &\gamma_3 = r_1 t_2 + r_2 t_1 = 0, \\ &\gamma_4 = r_1 t_3 + r_2 t_2 + r_3 t_1 = \\ &\frac{1}{64 d_1^3}\{d_1 d_3[12a_{nl}(a_{nl}-1)(20a_{nl}^2 + 25 - 12l(l+1))] \\ &+ d_2^2[(12a_{nl}^2 - 4l(l+1)+3)^2 + a_{nl}(5a_{nl}-3)(-68a_{nl}^2 + 36l(l+1) - 67)]\} \end{aligned} \quad (20)$$

and

$$\begin{aligned} &\gamma_5 = r_1 t_4 + r_2 t_3 + r_3 t_2 + r_4 t_1 = \\ &-\frac{(-d_1)^{1/2}}{8^3 d_1^5} \left\{6 d_1 d_2 d_3 \left[q_{nl}^{(1)} + q_{nl}^{(2)} + q_{nl}^{(3)}\right] + d_2^3 \left[q_{nl}^{(4)} + q_{nl}^{(5)}\right]\right\} \end{aligned} \quad (21)$$

where

$$
\begin{aligned}
q_{nl}^{(1)} &= -8a_{nl}^3[110a_{nl}^2 - 84l(l+1) + 295] \\
q_{nl}^{(2)} &= -3a_{nl}[4l(l+1) - 3][4l(l+1) - 35] \\
q_{nl}^{(3)} &= 2(1 + a_{nl})[12a_{nl}^2 - 4l(l+1) + 3][20a_{nl}^2 - 12l(l+1) + 25] \\
q_{nl}^{(4)} &= 24a_{nl}^3[250a_{nl}^2 - 172l(l+1) + 569] \\
q_{nl}^{(5)} &= a_{nl}[4l(l+1) - 3][44l(l+1) - 513] + \\
&(3 + 5a_{nl})[12a_{nl}^2 - 4l(l+1) + 3][-68a_{nl}^2 + 36l(l+1) - 67]
\end{aligned}
\tag{22}
$$

Therefore, the result for the dimensionless product P_{nl} is:

$$
P_{nl} \equiv \frac{< r^2 >_{nl} < p^2 >_{nl}}{\hbar^2} =
$$

$$
(2n + l + \frac{3}{2})^2 + \gamma_4 s^2 + \gamma_5 s^3 + \vartheta(s^4) \equiv P_{nl}^{(0)} + P_{nl}^{(2)} + P_{nl}^{(3)} + \vartheta(s^4) \tag{23}
$$

It is seen that the structure of the dimensionless product is fairly simple, but the coefficients γ_k become progressively more complicated as the power of s increases. It is further seen that there is no contribution of terms proportional to the small dimensionless quantity s but of terms of s^2 and higher.

3. Numerical values of the dimensionless product P_{nl} and discussion

In this section we report the numerical results obtained with the derived expression (23) of the dimensionless product P_{nl} for the first bound states and the various values of the small quantity s. Each contribution to P_{nl} : $P_{nl}^{(0)}$, $P_{nl}^{(2)}$ and $P_{nl}^{(3)}$ is also given in each case. The detailed results obtained with the PT potential are given in tables 1-4, while those with the Gaussian potential are displayed in ref.[20], where it is seen that the corresponding P_{nl} values are a little larger.

Numerical values of the dimensionless product P_{nl} and the partial contributions $P_{nl}^{(j)}$ to it for the states nl=00,10,01,02, (tables 1,2,3 and 4, respectively) for various values of s. The (reduced) PT potential was used.

Table 1.

s	$P_{00}^{(0)}$	$P_{00}^{(2)}$	$P_{00}^{(3)}$	P_{00}
0.00	2.250	0	0	2.2500
0.02	2.250	0.00014	0.00001	2.2501
0.04	2.250	0.00055	0.00004	2.2506
0.06	2.250	0.00124	0.00014	2.2514
0.08	2.250	0.00220	0.00033	2.2525
0.10	2.250	0.00344	0.00064	2.2541
0.12	2.250	0.00495	0.00110	2.2561

Table 2.

s	$P_{10}^{(0)}$	$P_{10}^{(2)}$	$P_{10}^{(3)}$	P_{10}
0.00	12.250	0	0	12.2500
0.02	12.250	-0.00256	-0.00021	12.2472
0.04	12.250	-0.01025	-0.00167	12.2381
0.06	12.250	-0.02306	-0.00565	12.2213
0.08	12.250	-0.04100	-0.01339	12.1956
0.10	12.250	-0.06462	-0.02616	12.1598
0.12	12.250	-0.09225	-0.04520	12.1126

Table 3.

s	$P_{01}^{(0)}$	$P_{01}^{(2)}$	$P_{01}^{(3)}$	P_{01}
0.00	6.250	0	0	6.2500
0.02	6.250	0.00071	0.00005	6.2508
0.04	6.250	0.00284	0.00037	6.2532
0.06	6.250	0.00639	0.00126	6.2577
0.08	6.250	0.01136	0.00299	6.2644
0.10	6.250	0.01774	0.00584	6.2736
0.12	6.250	0.02555	0.01009	6.2856

Table 4.

s	$P_{02}^{(0)}$	$P_{02}^{(2)}$	$P_{02}^{(3)}$	P_{02}
0.00	12.250	0	0	12.2500
0.02	12.250	0.00324	0.00026	12.2535
0.04	12.250	0.01295	0.00206	12.2650
0.06	12.250	0.02914	0.00697	12.2861
0.08	12.250	0.05180	0.01651	12.3183
0.10	12.250	0.08094	0.03224	12.3632
0.12	12.250	0.11655	0.05572	12.4223

It is clear from the results obtained in all tables that the main contribution to P_{nl}, for each bound state, comes from the corresponding zeroth order term $P_{nl}^{(0)}$ (see expression (23)). This is more pronounced for the ground state (n=0,l=0) and the smaller values of s, as is expected. It is also noted that the (absolute) values of $P_{nl}^{(3)}$ are smaller than the corresponding ones of $P_{nl}^{(2)}$ and often the difference between the two values is quite substantial.

On the basis of the above observations, it is therefore seen that the values of the dimensionless product P_{nl} are quite close to the corresponding values of the harmonic oscillator potential $P_{nl}^{(HO)} = P_{nl}^{(0)}$. This fact corroborates the suitability of the terminology of the potentials of this class as "oscillator-like" potentials. Pertaining to other types of potentials, such as the Coulomb and the spherically symmetric rectangular infinite well for which exact analytic results exist:

$$P_{nl}^{C} = \frac{1}{2}[5n^2 + 1 - 3l(l+1)] \tag{24}$$

and

$$P_{nl}^{IW} = \frac{1}{3}[X_{nl}^2 + \frac{1}{2}(2l+3)(2l-1)] \tag{25}$$

(X_{nl} being the roots of the l-th order spherical Bessel function), the corresponding values of P_{nl} are quite different [20].

It is clear, since $s = (\frac{\hbar^2}{2\mu V_0 R^2})^{1/2}$, that small values of s imply deep (large V_o) and wide (large R) potential wells. An interesting physical system corresponding to the situation of a wide well, (for which are known experimentally certain energy eigenvalues) is a rather heavy Λ-hypernucleus. The self-consistent field felt by the Λ-particle in the hypernucleus is very complicated,

but suitable single-particle potentials can be used often very satisfactorily. Two-parameter central potentials of the type used here may be considered as possible candidates for a rough representation of a more realistic single-particle potential. These potentials are in their turn, more realistic than the well-known harmonic oscillator potential, which because of its considerable analytic advantages has been very popular in Nuclear Physics problems for purposes of rough estimates. The use of the HVT technique has shown that potentials of the class considered can be useful in a number of cases for these purposes [18,19]. To guarantee rather small values of s one should consider, however, hypernuclei with fairly large mass numbers.

In conclusion, the present work shows that the HVT technique provides for sufficiently small values of s, a rather simple and handy way to estimate the dimensionless product P_{nl} for any (deeply) bound eigenstate of a wide class of central single particle hamiltonians, treating them in a unified way.

Acknowledgements The authors would like to thank Prof. S. Massen and Dr. K. Ypsilantis for useful technical advice and assistance. One of the authors (K.J.O.) is thankful to the Aristotle University of Thessaloniki for a scholarship which made possible to him a short term visit to the School of Physics of this University.

References

[1] J.O. Hirschfelder, Chem. Phys. 33 1462 (1960)

S.M. McRae and E.R. Vrscay, J. Math. Phys. 33 3004 (1992)

F.M. Fernandez and D.A. Castro, *Hypervirial Theorems (Lecture Notes in Chemistry* vol 43) (Berlin: Springer)

[2] J. Killingbeck, Phys. Lett. A**65**, 87 (1978)

J. Killingbeck, Microcomputer Quantum Mechanics, 1983 (Bristol, Hilger) ch 9 and references therein

[3] M. Grant and C.S. Lai, Phys. Rev. A20, 718 (1979)

C.S. Lai, Phys. Rev. A23, 445 (1981)

C.S. Lai and Lin, J. Phys. A Math. Gen. 24, 5291 (1991)

[4] Th.E. Liolios and M.E. Grypeos, International Journal of Theoretical Physics 2051 (1997)

Th.E. Liolios Computer Physics Communications 105,254 (1997)

Th. E. Liolios, Ph. D. thesis, University of Thessaloniki (1997)

[5] M.E. Grypeos and Th. Liolios, Phys. Let. A252, 125 (1999))

[6] R.J. Swenson and S.H. Danforth, J. Chem. Phys. 57 (1972)

[7] R.P. Feynmann, Phys. Rev. 56, 340 (1930)

H. Hellmann, Einfuhrung in die Quantenchemie, Deuticko, Vienna (1937)

[8] M.E. Grypeos, C.G. Koutroulos, Th.A. Petridou, J. Phys. A: Math. Gen. 35, 2233 (2002)

[9] R.G. Lombard, S. Marcos and J. Mares, Phys. Rev. C50, 2900 (1994)

[10] W. Thirring, A course in Mathematical Physics 3. Quantum Mechanics of Atoms and Molecules (Springer, New York) (1979)

[11] R.A. Bertlmann and A. Martin, Nucl. Phys. B168, 111 (1980)

[12] W. Heisenberg, Z. Phys. 43, 172 (1927)

[13] M.J.W. Hall, Phys. Rev. A64 052103 and references therein

[14] a) V.V. Dodonov, V.I. Man'ko, Generalization of the Uncertainty relations in Quantum Mechanics, Proceedings of the Lebedev Science Institute, Vol. 183, Nova Science Publ., N.Y. 1989

b) M.M. Nieto, Phys. Rev. A20, 700 (1979)

[15] J. Killingbeck, J. Phys. A Math. Gen. 14, 1005 (1981)

J. Killingbeck, J. Phys. A Math. Gen. 20, 601 (1987)

[16] M.R.M. Witwit, J. Phys. A, Math. Gen. 24, 3041 (1991)

M.R.M. Witwit, J. Phys. A, Math. Gen. 24, 3053 (1991)

M.R.M. Witwit, J. Phys. A, Math. Gen. 24, 4535 (1991)

[17] J. Killingbeck, G. Jolicard, Chem. Phys. Lett. 284, 359 (1998)
J. Killingbeck, A. Grosjean, J.M. Zucconi, Phys. Lett. A261 169 (1999)

[18] Th.E. Liolios, Eur. Phys. J. A4 329 (1999)

[19] M.E. Grypeos, C.G. Koutroulos, Th.A. Petridou, Int.J. Mod. Phys. E10, 393 (2001)

[20] M.E. Grypeos, C.G. Koutroulos, K.J. Oyewumi, Th. Petridou, submitted for publication.