Study of a class of non-polynomial oscillator potentials

Nasser Saad[1]**, Richard L Hall**[2] **and Hakan Ciftci**[3]

[1] Department of Mathematics and Statistics, University of Prince Edward Island,
550 University Avenue, Charlottetown, PEI, C1A 4P3, Canada
[2] Department of Mathematics and Statistics, Concordia University, 1455 de Maisonneuve
Boulevard West, Montréal, Québec H3G 1M8, Canada
[3] Gazi Universitesi, Fen-Edebiyat Fakültesi, Fizik Bölümü, 06500 Teknikokullar, Ankara, Turkey

Abstract
We develop a variational method to obtain accurate bounds for the eigenenergies
of $H = -\Delta + V$ in arbitrary dimensions $N > 1$, where $V(r)$ is the
nonpolynomial oscillator potential $V(r) = r^2 + \frac{\lambda r^2}{1+gr^2}$, $\lambda \in (-\infty, \infty)$, $g > 0$.
The variational bounds are compared with results previously obtained in the
literature. An infinite set of exact solutions is also obtained and used as a source
of comparison eigenvalues.

PACS number: 03.65.Ge

1. Introduction

The following is a variational study of the eigenvalues of the Hamiltonian $H = \Delta + V(r)$,
where the non-polynomial oscillator potential $V(r)$ is given in arbitrary dimensions by

$$V(r) = r^2 + \frac{\lambda r^2}{1 + gr^2}, \qquad g > 0, \quad \lambda \in (-\infty, \infty). \qquad (1.1)$$

Various techniques may be found in the literature [1–53] for the estimation of the spectrum
corresponding to this potential. Some of these techniques have been developed only for
special values of λ and g. The purpose of the present work is to introduce a unified variational
technique to compute the eigenvalues of Schrödinger's equation with potential (1.1) in arbitrary
dimension $N > 1$ and for arbitrary angular quantum number $l = 0, 1, 2, \ldots$. The variational
method presented here has the advantage of being valid for arbitrary values of λ, $g > 0$
in arbitrary dimension N. The paper is organized as follows. In section 2, we introduce a
variational technique based on the Gol'dman and Krivchenkov Hamiltonian as a solvable
model. Thereafter, we use its eigensolutions to compute the matrix elements for the operators
$r^2/(1 + gr^2)$, $g > 0$. Closed-form analytic expressions in terms of the incomplete gamma
function are obtained for the matrix elements. In section 3, application to the non-polynomial
oscillator potential is discussed and we compare our results with those by other techniques
available in the literature. Some remarks regarding the perturbation expansions are also given

in section 4. Our conclusions are presented in section 4. For comparison, we review, in the appendix, the exact solutions of the Schrödinger equation with the potential (1.1) valid for certain relations between the parameters λ and g. These exact solutions are valid for $\lambda < 0$ and can be seen as generalizations of the exact solutions in the one-dimensional case developed earlier in the literature. The purpose of exploring these exact solutions is to use them for testing the accuracy of the variational method we develop in section 2.

2. Variational approximation by means of an exactly solvable model

The radial Schrödinger equation in N-space dimension for the nth quantum state of the non-polynomial oscillator potential (1.1) can be written, with $\hbar/2m = 1$, as

$$H\phi_{nl}^N(r) = \left(-\frac{d^2}{dr^2} + Br^2 + \frac{\left(l + \frac{1}{2}(N-3)\right)\left(l + \frac{1}{2}(N-1)\right)}{r^2} + \frac{\lambda r^2}{1 + gr^2} \right)\phi_{nl}^N(r) = E_{nl}^N\phi_{nl}^N(r), \tag{2.1}$$

where $l = 0$ for the $N = 1$ case. Here the parameter B is introduced to simplify the computation of the matrix elements of H; it may be set equal to 1 afterwards, without disturbing the computation. For $N > 1$, n refers to the radial quantum number (that is to say, $n - 1$ is the number of radial nodes). For certain relations between the parameters λ and g, exact solutions can be obtained [22, 23, 31, 32, 35, 36, 38, 39]. These exact solutions are summarized in the appendix and are valid for arbitrary values of $\gamma = l + \frac{1}{2}(N - 3)$, i.e. not restricted to certain integer values of N and l as reported in the literature. They will be used to verify the numerical computations by the variational technique we are about to develop. Our variational approach is based on the introduction of a dummy variational parameter A on which the full perturbation expansion does not depend (though the truncated expansion does). The optimal value of the variational parameter is then determined by a minimization process. Let us write the Hamiltonian H in (2.1) as

$$H = H_0 + \left(\frac{\lambda r^2}{1 + gr^2} - \frac{A}{r^2} \right), \qquad A \geqslant -\frac{1}{4} \tag{2.2}$$

where

$$H_0 = -\frac{d^2}{dr^2} + Br^2 + \frac{\left(l + \frac{1}{2}(N-3)\right)\left(l + \frac{1}{2}(N-1)\right) + A}{r^2}, \qquad l = 0, 1, 2, \ldots. \tag{2.3}$$

The unperturbed Hamiltonian H_0, known as the Gol'dman and Krivchenkov Hamiltonian, is one of the few systems that admit exact analytical solutions [54]. It is the generalization of the familiar harmonic oscillator in three dimension $-d^2/dr^2 + Br^2 + l(l+1)/r^2$, where the generalization lies in the parameter A ranging over $[-\frac{1}{4}, \infty)$ instead of only values determined by the angular momentum quantum numbers $l = 0, 1, 2, \ldots$. The energy spectrum of the Schrödinger equation $H_0\psi_{nl}^N = \epsilon_{nl}^N\psi_{nl}^N$ is given, in terms of parameters A and B, by

$$\epsilon_{nl}^N = 2\beta(2n + \zeta), \quad n = 0, 1, 2, \ldots, \quad \left(\beta = \sqrt{B}, \zeta = 1 + \sqrt{A + \left(l + \frac{N}{2} - 1\right)^2} \right) \tag{2.4}$$

where the *normalized* wavefunctions are given explicitly by

$$\psi_{nl}^N(r) = (-1)^n \sqrt{\frac{2\beta^\zeta(\zeta)_n}{n!\Gamma(\zeta)}} r^{\zeta - \frac{1}{2}} e^{-\frac{\beta}{2}r^2} {}_1F_1\left(\begin{matrix} -n \\ \zeta \end{matrix} \middle| \beta r^2 \right), \qquad (n, l = 0, 1, 2, \ldots, N > 1). \tag{2.5}$$

The confluent hypergeometric function $_1F_1$ is defined by means of the polynomial

$$_1F_1\left(\begin{matrix}-n\\b\end{matrix}\middle|z\right) = \sum_{k=0}^{n} \frac{(-n)_k z^k}{(b)_k k!}, \qquad (n\text{-degree polynomial in } z) \tag{2.6}$$

where the shifted factorial $(a)_n$ is defined by

$$(a)_0 = 1, \qquad (a)_n = a(a+1)(a+2)\dots(a+n-1), \qquad \text{for} \quad n = 1, 2, 3, \dots. \tag{2.7}$$

The singular basis, consisting of the set of exact solutions of H_0, serves as a good starting point for the analysis of the non-polynomial oscillator Hamiltonian H given in (2.1). Indeed, the use of the basis (2.5) will allow us to overcome the difficulties which arise if one uses Hermite functions [41]. The matrix elements of the Hamiltonian H, (2.2), in terms of the orthonormal basis (2.5), read

$$\langle\psi_{ml}^N|H|\psi_{nl}^N\rangle = 2(2n+\zeta)\delta_{mn} + \langle\psi_{ml}^N|\frac{\lambda r^2}{1+gr^2}|\psi_{nl}^N\rangle - \langle\psi_{ml}^N|Ar^{-2}|\psi_{nl}^N\rangle, \tag{2.8}$$

where the Kronecker delta $\delta_{mn} = 0$ for $m \neq n$ and 1 for $m = n$. Consequently, to make use of the matrix elements (2.8), we need to evaluate the expectation values $\langle\psi_{ml}^N|\frac{r^2}{1+gr^2}|\psi_{nl}^N\rangle$ and $\langle\psi_{ml}^N|r^{-2}|\psi_{nl}^N\rangle$ by means of the orthonormal basis (2.5). This is summarized by the following two theorems.

Theorem 1. *By means of the orthonormal basis $\{\psi_{nl}^N\}_{n=0}^{\infty}$, where $\psi_{nl}^N(r)$ is given by (2.5), we have*

$$\langle\psi_{ml}^N|\frac{r^2}{1+gr^2}|\psi_{nl}^N\rangle \equiv \int_0^{\infty} \frac{r^2\psi_{ml}^N(r)\psi_{nl}^N(r)}{1+gr^2}\,\mathrm{d}r = (-1)^{m+n}\frac{\beta^\zeta\, \mathrm{e}^{\beta/g}}{g^{\zeta+1}\Gamma(\zeta)}\sqrt{\frac{(\zeta)_n(\zeta)_m}{n!m!}}$$
$$\times \sum_{i=0}^{n}\sum_{j=0}^{m}\frac{(-n)_i(-m)_j}{(\zeta)_i(\zeta)_j i! j!}\left(\frac{\beta}{g}\right)^{i+j}\Gamma(\zeta+i+j+1)\Gamma\left(-\zeta-i-j;\frac{\beta}{g}\right). \tag{2.9}$$

Here $\Gamma\left(-\zeta-i-j;\frac{\beta}{g}\right)$ is the incomplete gamma function defined by $\Gamma(a,z) = \int_z^{\infty} t^{a-1}\,\mathrm{e}^{-t}\,\mathrm{d}t$.

Proof. Direct integration of $\int_0^{\infty}\frac{r^2\psi_{nl}^N(r)\psi_{nl}^N(r)}{1+gr^2}\,\mathrm{d}r$ using (2.5) yields

$$\int_0^{\infty} \frac{r^2\psi_{ml}^N(r)\psi_{nl}^N(r)}{1+gr^2}\,\mathrm{d}r = \frac{2(-1)^{m+n}\beta^\zeta}{\Gamma(\zeta)}\sqrt{\frac{(\zeta)_n(\zeta)_m}{n!m!}}$$
$$\times \int_0^{\infty}\frac{r^{2\zeta+1}\,\mathrm{e}^{-\beta r^2}}{1+gr^2}\,_1F_1\left(\begin{matrix}-n\\\zeta\end{matrix}\middle|\beta r^2\right){_1F_1}\left(\begin{matrix}-m\\\zeta\end{matrix}\middle|\beta r^2\right)\mathrm{d}r$$
$$= \frac{2(-1)^{m+n}\beta^\zeta}{\Gamma(\zeta)}\sqrt{\frac{(\zeta)_n(\zeta)_m}{n!m!}}\sum_{i=0}^{n}\sum_{j=0}^{m}\frac{(-n)_i(-m)_j\beta^{i+j}}{(\zeta)_i(\zeta)_j i! j!}$$
$$\times \int_0^{\infty}\frac{r^{2\zeta+2i+2j+1}}{1+gr^2}\,\mathrm{e}^{-\beta r^2}\,\mathrm{d}r \tag{2.10}$$

where we have used the terminated series representation of the confluent hypergeometric function (2.6). The question is now reduced to the computation of the finite integral

$$I(\beta) = \int_0^{\infty}\frac{r^{2\zeta+2i+2j+1}}{1+gr^2}\,\mathrm{e}^{-\beta r^2}\,\mathrm{d}r = \frac{1}{2}\int_0^{\infty}\frac{x^{\zeta+i+j}}{1+gx}\,\mathrm{e}^{-\beta x}\,\mathrm{d}x, \quad \text{(after substituting } r^2 = x\text{)}.$$
$$\tag{2.11}$$

Such an integral has been questioned in the literature [5, 9, 14, 28, 41]; therefore, we shall give a detail calculation of it here. Differentiation of (2.11) with respect to β yields

$$\frac{\mathrm{d}I(\beta)}{\mathrm{d}\beta} = -\frac{1}{2} \int_0^\infty \frac{x^{\zeta+i+j+1}}{1+gx} \, \mathrm{e}^{-\beta x} \, \mathrm{d}x. \tag{2.12}$$

Multiplying (2.12) by g and subtracting it from (2.11) implies

$$I(\beta) - g\frac{\mathrm{d}I(\beta)}{\mathrm{d}\beta} = \frac{1}{2} \int_0^\infty x^{\zeta+i+j} \, \mathrm{e}^{-\beta x} \, \mathrm{d}x.$$

The integral on the right-hand side can be easily calculated by using the definition of the gamma function $\Gamma(z) = \int_0^\infty \mathrm{e}^{-t} t^{z-1} \, \mathrm{d}t$, $\mathrm{Re}(z) > 0$, and yields

$$I(\beta) - g\frac{\mathrm{d}I(\beta)}{\mathrm{d}\beta} = \frac{1}{2}\beta^{-(\zeta+i+j+1)}\Gamma(\zeta+i+j+1).$$

This is an elementary first-order differential equation which can be easily solved as

$$I(\beta) = \frac{1}{\mathrm{e}^{-\frac{\beta}{g}}}\left[-\frac{\Gamma(\zeta+i+j+1)}{2g} \int_{\epsilon>0}^\beta \mathrm{e}^{-\frac{\eta}{g}} \eta^{-(\zeta+i+j+1)} \, \mathrm{d}\eta + C \right],$$

where the constant C is chosen such that $I(\beta) \to 0$ as $\beta \to \infty$ (a conclusion which follows from the definition of the Laplace transform). Therefore, we have, after simple algebra and use of L'Hospital's rule, that

$$I(\beta) = \frac{\Gamma(\zeta+i+j+1)}{2g\,\mathrm{e}^{-\frac{\beta}{g}}} \int_\beta^\infty \mathrm{e}^{-\frac{\eta}{g}} \eta^{-(\zeta+i+j+1)} \, \mathrm{d}\eta = \frac{\Gamma(\zeta+i+j+1)}{2g^{\zeta+i+j+1}\,\mathrm{e}^{-\frac{\beta}{g}}} \int_{\frac{\beta}{g}}^\infty \mathrm{e}^{-\eta} \eta^{-(\zeta+i+j+1)} \, \mathrm{d}\eta$$

which is the definition of the incomplete gamma function. This completes the proof. $\qquad\square$

Theorem 2. *By means of (2.5), we have*

$$\langle \psi_{ml}^N | r^{-2} | \psi_{nl}^N \rangle = \begin{cases} (-1)^{m+n} \frac{\beta}{\zeta-1} \sqrt{\frac{n!(\zeta)_m}{m!(\zeta)_n}} & \text{if} \quad n > m, \\ \frac{\beta}{\zeta-1} & \text{if} \quad n = m, \\ (-1)^{m+n} \frac{\beta}{\zeta-1} \sqrt{\frac{m!(\zeta)_n}{n!(\zeta)_m}} & \text{if} \quad n < m. \end{cases} \tag{2.13}$$

Proof. Direct integration of $\int_0^\infty r^{-2} \psi_{nl}^N(r) \psi_{nl}^N(r) \, \mathrm{d}r$ using (2.5) yields

$$\langle \psi_{nl}^N(r) | r^{-2} | \psi_{nl}^N(r) \rangle = \frac{2(-1)^{m+n}\beta^\zeta}{\Gamma(\zeta)} \sqrt{\frac{(\zeta)_n(\zeta)_m}{nm!}}$$

$$\times \int_0^\infty r^{2\zeta-3} \, \mathrm{e}^{-\beta r^2} {}_1F_1(-n;\zeta;\beta r^2) {}_1F_1(-m;\zeta;\beta r^2) \, \mathrm{d}r.$$

The finite integral on the right-hand side follows directly by means of the identity [54]

$$\int_0^\infty r^{2\zeta-\alpha-1} \, \mathrm{e}^{-\beta r^2} {}_1F_1\left(\begin{matrix} -n \\ \zeta \end{matrix} \middle| \beta r^2 \right) {}_1F_1\left(\begin{matrix} -m \\ \zeta \end{matrix} \middle| \beta r^2 \right) \, \mathrm{d}r$$

$$= \frac{\left(\frac{\alpha}{2}\right)_n \Gamma\left(\zeta-\frac{\alpha}{2}\right)}{2\beta^{\zeta-\frac{\alpha}{2}}(\zeta)_n} {}_3F_2\left(\begin{matrix} -m, \zeta-\frac{\alpha}{2}, 1-\frac{\alpha}{2} \\ \zeta, 1-\frac{\alpha}{2}-n \end{matrix} \middle| 1 \right). \tag{2.14}$$

The proof of the theorem then follows from the fact that the hypergeometric function

$$_3F_2\left(\begin{matrix} -m, a, b \\ c, d \end{matrix} \middle| 1 \right) = \sum_{k=0}^m \frac{(-m)_k(a)_k(b)_k}{(c)_k(d)_k k!}, \qquad (m\text{-degree polynomial}).$$

collapses to unity when $\alpha = 2$. $\qquad\square$

Theorems 1 and 2 provide closed-form analytic expressions for the matrix elements (2.8); these allow us to obtain accurate upper bounds for the Hamiltonian (2.1) by means of the following optimization problem:

$$E_{nl}^N \leqslant \min_{A \geqslant -\frac{1}{4}} \mathrm{diag} \begin{pmatrix} H_{00} & H_{01} & \ldots & H_{0D-1} \\ H_{10} & H_{11} & \ldots & H_{1D-1} \\ \ldots & \ldots & \ldots & \ldots \\ H_{D-10} & H_{D-11} & \ldots & H_{D-1D-1} \end{pmatrix}, \qquad H_{mn} = \langle \psi_{ml}^N | H | \psi_{nl}^N \rangle, \quad (2.15)$$

for fixed B.

3. Applications and numerical results

In order to avoid the numerical complication [55] of computing the incomplete gamma functions in (2.8), we have, by means of the recurrence relation [56]

$$\Gamma(a+1, z) = a\Gamma(a, z) + z^a \, \mathrm{e}^{-z}, \qquad (3.1)$$

that

$$\Gamma(a, z) = \frac{\Gamma(a+n, z)}{(a)_n} - \mathrm{e}^{-z} \sum_{k=1}^{n} \frac{z^{a+k-1}}{(a)_k}. \qquad (3.2)$$

Thus

$$\Gamma\left(-\zeta - i - j, \frac{\beta}{g}\right) = \frac{(-1)^{i+j} \Gamma\left(-\zeta, \frac{\beta}{g}\right)}{(1+\zeta)_{i+j}} - \left(\frac{g}{\beta}\right)^{\zeta+i+j+1} \mathrm{e}^{-\frac{\beta}{g}} \sum_{k=1}^{i+j} \frac{\left(\frac{\beta}{g}\right)^k}{(-\zeta - i - j)_k}. \qquad (3.3)$$

Consequently, (2.9) now becomes

$$\langle \psi_{ml}^N | \frac{r^2}{1+gr^2} | \psi_{nl}^N \rangle = (-1)^{m+n} \frac{\zeta \beta^\zeta \, \mathrm{e}^{\beta/g}}{g^{\zeta+1}} \sqrt{\frac{(\zeta)_n (\zeta)_m}{n! m!}} \Gamma\left(-\zeta, \frac{\beta}{g}\right) \sum_{i=0}^{n} \sum_{j=0}^{m} \frac{(-n)_i (-m)_j}{(\zeta)_i (\zeta)_j i! j!} \left(-\frac{\beta}{g}\right)^{i+j}$$

$$- \frac{(-1)^{m+n}}{\beta \Gamma(\zeta)} \sqrt{\frac{(\zeta)_n (\zeta)_m}{n! m!}} \sum_{i=0}^{n} \sum_{j=0}^{m} \sum_{k=1}^{i+j} \frac{(-n)_i (-m)_j \Gamma(\zeta+i+j+1-k)}{(\zeta)_i (\zeta)_j i! j!} \left(-\frac{\beta}{g}\right)^k, \qquad (3.4)$$

where we have used the identity $(-\zeta - i - j)_k = \frac{(-1)^k}{(\zeta+i+j+1)_{-k}}$. The double sum of the first term on the right-hand side of (3.4) can be written in terms of the confluent hypergeometric function (2.6). In this case, we have

$$\langle \psi_{ml}^N | \frac{r^2}{1+gr^2} | \psi_{nl}^N \rangle = (-1)^{m+n} \frac{\zeta \beta^\zeta \, \mathrm{e}^{\beta/g}}{g^{\zeta+1}} \sqrt{\frac{(\zeta)_n (\zeta)_m}{n! m!}} \Gamma\left(-\zeta, \frac{\beta}{g}\right)$$

$$\times {}_1F_1\left(\begin{matrix} -n \\ \zeta \end{matrix} \middle| -\frac{\beta}{g}\right) {}_1F_1\left(\begin{matrix} -m \\ \zeta \end{matrix} \middle| -\frac{\beta}{g}\right) - \frac{(-1)^{m+n}}{\beta \Gamma(\zeta)} \sqrt{\frac{(\zeta)_n (\zeta)_m}{n! m!}}$$

$$\times \sum_{i=0}^{n} \sum_{j=0}^{m} \sum_{k=1}^{i+j} \frac{(-n)_i (-m)_j \Gamma(\zeta+i+j+1-k)}{(\zeta)_i (\zeta)_j i! j!} \left(-\frac{\beta}{g}\right)^k. \qquad (3.5)$$

The advantage of using such expressions as (3.4) or (3.5) is that they allow us to compute the incomplete gamma function only once, since its parameters are fixed. In our numerical computations of the variational upper bounds, we shall use (3.4) which can be implemented using symbolic mathematical software such as Mathematica or Maple. In order to verify the

Table 1. Comparison of the exact eigenvalues obtained by means of (3.6) and that obtained by the variational technique E_{var} discussed in the present work. The number D in the square brackets refers to the size of the basis set used in this case.

g	γ	λ	E_{exact}	E_{var}
0.1	0	-0.46	2.400 000 000 000	2.400 000 000 000 [2]
	2	-0.54	5.600 000 000 000	5.600 000 000 000 [2]
1	0	-10.0	$-3.000\,000\,000\,000$	$-3.000\,000\,000\,000$ [2]
	2	-18.0	$-7.000\,000\,000\,000$	$-7.000\,000\,000\,000$ [2]
10	0	-640	$-57.000\,000\,000\,000$	$-57.000\,000\,000\,000$ [2]
	2	-1440	$-133.000\,000\,000\,000$	$-133.000\,000\,000\,000$ [2]

usefulness of this variational approach, as well as its generality for computing upper bounds for arbitrary values of the parameters λ and $g > 0$, we will now compare our results with the exact eigenvalues obtained for certain relations of the parameters (as summarized in the appendix) and with the most recent approximate eigenvalues obtained in the literature by means of a variety of techniques.

3.1. Comparison with exact solutions

We first compare the variational upper bounds with the exact solutions developed in the appendix. It is known [24] that such exact solutions are only possible for $\lambda < 0$ and for certain algebraic relations between the parameters λ and g. For the Schrödinger equation (2.1) with $\gamma = l + \frac{1}{2}(N - 3)$ or real number $\gamma \geqslant -1$ and $B = 1$, we have using (A.4) for $n = 1$ that

$$H\psi = -\frac{d^2\psi}{dr^2} + \left(r^2 + \frac{\gamma(\gamma + 1)}{r^2} - \frac{4g + 2g^2(3 + 2\gamma)}{1 + gr^2}\right)\psi = (3 + 2\gamma)(1 - 2g)\psi \qquad (3.6)$$

with the exact nodeless ground state $\psi(r) = r^{\gamma+1}(1 + gr^2)\,e^{-r^2/2}$. In this case, the variational method for computing the upper bound of H in (3.6) converges rapidly for arbitrary values of $g > 0$ and minimization of 2×2 matrix (2.15) over A is sufficient to obtain very accurate upper bounds, as indicated by table 1, in comparison with the exact eigenvalues given by (3.6). Further, from (A.4) for $n = 2$, we note that for $\lambda = (E_\pm - 2\gamma - 11)g$ where

$$E_\pm = 5 + 2\gamma - g(13 + 6\gamma) \pm \sqrt{g^2(7 + 2\gamma)^2 + g(-4 + 8\gamma) + 4}, \qquad (3.7)$$

the corresponding eigenstates read

$$\psi_2^\pm(r) = r^{\gamma+1}(1 + gr^2)(1 + a_\pm r^2)\,e^{-r^2/2}, \qquad (3.8)$$

where

$$a_\pm = -\frac{E_\pm + (2g - 1)(3 + 2\gamma)}{(6 + 4\gamma)}.$$

For E_+, we have $a_+ < 0$ and the wavefunction $\psi_2^+(r)$ has one node on $[0, \infty)$; thus $\psi_2^+(r)$ is the eigenstate for the first excited state in this case. On the other hand, for E_-, $a_- > 0$ and the wavefunction $\psi_2^-(r)$ has no node and thus represents the ground-state wavefunction when g and λ satisfy the correspondence condition. In table 2, we have compared our variational results with those obtained by (3.7). It should be mentioned that these variational eigenvalues are obtained by optimizing (2.15) over a *two*-dimensional subspace. The best possible value of the free minimization parameter A is found to be zero.

Table 2. Comparison of the eigenvalues obtained by means of (3.7) and those obtained by the variational technique E_{var} discussed in the present work. The number D in the square brackets refers to the size of the basis set used in this case.

g	γ	λ	E_{exact}	E_{var}
0.1	0	-26	$-15.000\,000\,000\,000$	$-14.999\,999\,999\,999\,9$ [2]
		-12	$-1.000\,000\,000\,000$	$-0.999\,999\,999\,999\,96$ [2]
	1	$-0.561\,745\,755\,789\,733\,451\,89$	$7.382\,542\,442\,102\,665$	$7.382\,542\,442\,102\,671$ [2]
		$-1.018\,254\,244\,210\,266\,5481$	$2.817\,457\,557\,897\,335$	$2.817\,457\,557\,897\,341$ [2]

Table 3. Comparison of the convergence of the lowest two odd eigenvalues of the nonpolynomial oscillator Hamiltonian $-\mathrm{d}^2/\mathrm{d}r^2 + r^2 + r^2/(1+gr^2)$ between the variational method proposed in the present paper and the quadrature discretization method (QDM) [57] with different weight functions $w(r)$. The number D in the square brackets refers to the size of the basis set used in each method.

g	n	E_{var}	E_{QDM} $w(r) = \mathrm{e}^{-\alpha r^2}$	E_{QDM} $w(r) = \mathrm{e}^{-r^2\sqrt{1+\lambda/(1+0.5g)}}$
1	1	$3.511\,580\,94$ [$D=1$]	$3.510\,993\,89$ [$D=10$]	$3.506\,663\,67$ [$D=10$]
		$3.507\,406\,82$ [$D=5$]	$3.507\,388\,72$ [$D=20$]	$3.507\,375\,73$ [$D=20$]
		$3.507\,388\,65$ [$D=10$]	$3.507\,388\,37$ [$D=25$]	$3.507\,387\,81$ [$D=30$]
		$3.507\,388\,36$ [$D=15$]	$\underline{3.507\,388\,35}$ [$D=30$]	$3.507\,388\,31$ [$D=40$]
		$\underline{3.507\,388\,35}$ [$N=16$]	$3.507\,388\,35$ [$D=30$]	$3.507\,388\,35$ [$D=50$]
	2	$7.652\,201\,93$ [$D=1$]	$7.838\,016\,90$ [$D=10$]	$7.645\,620\,64$ [$D=10$]
		$7.648\,282\,94$ [$D=5$]	$7.648\,364\,79$ [$D=20$]	$7.648\,153\,36$ [$D=20$]
		$7.648\,202\,50$ [$D=10$]	$7.648\,204\,06$ [$D=25$]	$7.648\,199\,20$ [$D=30$]
		$7.648\,201\,29$ [$D=15$]	$\underline{7.648\,201\,24}$ [$D=30$]	$7.648\,201\,10$ [$D=40$]
		$\underline{7.648\,201\,24}$ [$D=19$]	$7.648\,201\,24$ [$D=35$]	$7.648\,201\,24$ [$D=60$]
10	1	$3.088\,093\,37$ [$D=1$]	$3.541\,689\,06$ [$D=10$]	$3.086\,922\,34$ [$D=10$]
		$3.088\,091\,39$ [$D=5$]	$3.088\,830\,73$ [$D=30$]	$3.087\,944\,08$ [$D=30$]
		$3.088\,090\,96$ [$D=10$]	$3.088\,091\,33$ [$D=50$]	$3.088\,056\,98$ [$D=50$]
		$3.088\,090\,88$ [$D=15$]	$\underline{3.088\,090\,85}$ [$D=60$]	$3.088\,090\,57$ [$D=150$]
		$\underline{3.088\,090\,86}$ [$D=19$]	$3.088\,090\,85$ [$D=70$]	$\underline{3.088\,090\,75}$ [$D=180$]
	2	$7.090\,376\,23$ [$D=1$]	$11.039\,786\,81$ [$D=10$]	$7.088\,385\,86$ [$D=10$]
		$7.090\,371\,44$ [$D=5$]	$7.136\,120\,19$ [$D=30$]	$7.090\,120\,96$ [$D=20$]
		$7.090\,370\,60$ [$D=10$]	$7.090\,481\,60$ [$D=50$]	$7.090\,312\,84$ [$D=50$]
		$7.090\,370\,46$ [$D=15$]	$7.090\,370\,53$ [$D=70$]	$7.090\,369\,93$ [$D=150$]
		$\underline{7.090\,370\,43}$ [$D=19$]	$\underline{7.090\,370\,41}$ [$D=80$]	$\underline{7.090\,370\,25}$ [$D=180$]
100	1	$3.009\,831\,772$ [$D=1$]	$6.612\,894\,99$ [$D=10$]	$3.009\,811\,39$ [$D=10$]
		$3.009\,831\,771$ [$D=5$]	$3.009\,878\,06$ [$D=100$]	$3.009\,827\,85$ [$D=100$]
		$3.009\,831\,771$ [$D=10$]	$3.009\,831\,81$ [$D=150$]	$3.009\,830\,06$ [$D=170$]
		$\underline{3.009\,831\,771}$ [$D=15$]	$\underline{3.009\,831\,77}$ [$D=170$]	$\underline{3.009\,83\,023}$ [$D=180$]
	2	$7.009\,844\,96$ [$D=1$]	$25.734\,168\,48$ [$D=10$]	$7.009\,813\,97$ [$D=10$]
		$7.009\,844\,95$ [$D=5$]	$7.014\,814\,72$ [$D=30$]	$7.009\,839\,00$ [$D=100$]
		$7.009\,844\,95$ [$D=10$]	$7.009\,856\,17$ [$D=50$]	$7.009\,841\,72$ [$D=150$]
		$\underline{7.009\,844\,95}$ [$D=15$]	$\underline{7.009\,845\,17}$ [$D=180$]	$\underline{7.009\,84\,261}$ [$D=180$]

3.2. Comparison with the quadrature discretization method

In table 3, we compare our upper bounds with that of Chen and Shizgal [57, 58] obtained by means of the quadrature discretization method (QDM). The QDM generally employs a discretized version of the Hamiltonian with respect to a set of points that correspond to the quadrature points associated with the chosen weight function. The distribution of the grid points is determined by the weight function, which controls the convergence of the eigenvalues

Table 4. Comparison of the variational upper bounds E_{var} with the upper and lower bounds E_{EMM} obtained by means of the eigenvalue moment method (EMM) [44]. The number D in the square brackets refers to the size of the basis set used in each method. The size of the basis set used in the variational method is set to be $D = 18$.

λ	g	l	E_{var}	E_{EMM}
0.1	0.1	1	5.186 373 002 931 507	$5.186\,373\,002\,9314 < E < 5.186\,373\,002\,9316$
		2	7.243 961 840 421 887	$7.243\,961\,840\,4138 < E < 7.243\,961\,840\,4260$
		3	9.294 359 110 874 627	$9.294\,359\,110\,863\,37 < E < 9.294\,359\,110\,881\,59$
0.1	0.5	1	5.100 857 624 300 696	$5.100\,842 < E < 5.100\,865$
		2	7.118 980 871 564 27	$7.118\,90 < E < 7.118\,901$
		3	9.131 812 401 691 521	$9.131\,799 < E < 9.131\,838$
0.1	1	1	5.065 569 521 783 354	$5.064\,28 < E < 5.066\,09$
		2	7.073 726 361 909 647	$7.0730 < E < 7.0744$
		3	9.078 911 720 303 639	$9.0787 < E < 9.078\,92$
0.5	1	1	5.893 595 152 339 402	$5.893\,595\,152\,339\,19 < E < 5.893\,595\,152\,339\,45$
		2	8.177 871 693 4677	$8.177\,871\,693\,435 < E < 8.177\,871\,693\,485$
		3	10.429 204 118 147 453	$10.429\,204\,118\,1366 < E < 10.429\,204\,118\,1548$
1	0.1	1	6.704 238 892 478 644	$6.704\,238\,892\,4777 < E < 6.704\,238\,892\,4788$
		2	9.261 914 780 826 569	$9.261\,914\,7807 < E < 9.261\,914\,7809$
		3	11.760 620 962 669 972	$11.760\,620\,962\,6312 < E < 11.760\,620\,962\,6917$
1	1	1	5.651 393 317 250 17	$5.6503 < E < 5.6521$
		2	7.734 828 042 923 58	$7.734 < E < 7.736$
		3	9.787 669 778 509 466	$9.7875 < E < 9.7881$
100	100	1	5.993 438 873 366 758	$- < E < 6.389$
		2	7.996 024 673 021 835	$7.9947 < E < 8.037\,800$
		3	9.997 153 638 602 487	$9.9969 < E < 10.0113$

and eigenfunctions. In table 3, we have compared our results with those of [57, 58] using the weight functions $\exp(-\alpha r^2)$ and $\exp(-r^2\sqrt{1 + \lambda/(1 + 0.5g)})$, where α is chosen by the authors for the fastest convergence. The underlined portion of each eigenvalue indicates the convergence to the number of significant figures obtained by [57, 58] and has been mentioned for the purpose of comparison; we may extend the convergence of the upper bounds obtained by the variational method by increasing the size of D in (2.15). The number D indicates the size of the diagonalized matrix used in the diagonalization process or/and the number of quadrature points used in the application of the QDM. The table clearly indicates the faster convergence of the eigenvalues by means of the variational method.

3.3. Comparison with the eigenvalue moment method

The eigenvalue moment method (EMM) is an effective and simple technique for generating converging lower and upper bounds to the low-lying discrete spectrum of multidimensional quantum Hamiltonians [19, 44]. The method, however, faced some difficulties in determining eigenenergies for certain Hamiltonian parameter values. For the non-polynomial oscillator potential (1.1), we have compared our variational results obtained by means of (2.15) with those of EMM [44]. As seen from the table, EMM is not adequate for large values of g, whereas the variational method developed here gives good results.

3.4. Some remarks about first-order perturbation expansions

The closed-form expressions for the matrix elements (2.9) can be used explicitly to express the first-order perturbation expansions for the perturbed Hamiltonian (2.1) for any dimension

Table 5. The first-order perturbation expansions of the lowest three eigenvalues for different values of g and valid for small values of λ. For comparison see [28].

g	$E_{00}^3 - 3$	$E_{10}^3 - 7$	$E_{20}^3 - 11$
0.5	$0.741\,907\,668\,608\,869\lambda$	$1.058\,912\,626\,973\,532\lambda$	$1.216\,304\,645\,477\,702\lambda$
1	$0.515\,744\,312\,282\,624\lambda$	$0.648\,934\,634\,510\,945\lambda$	$0.712\,059\,158\,182\,293\lambda$
2	$0.327\,839\,771\,209\,399\lambda$	$0.374\,239\,389\,891\,732\lambda$	$0.396\,830\,711\,146\,285\lambda$
5	$0.160\,824\,698\,125\,120\lambda$	$0.169\,855\,585\,054\,398\lambda$	$0.174\,677\,060\,833\,675\lambda$
10	$0.088\,111\,301\,584\,084\lambda$	$0.090\,376\,621\,370\,169\lambda$	$0.091\,681\,154\,216\,976\lambda$
20	$0.046\,566\,260\,901\,426\lambda$	$0.047\,083\,627\,877\,117\lambda$	$0.047\,401\,822\,090\,664\lambda$
100	$0.009\,831\,778\,572\,526\lambda$	$0.009\,844\,958\,882\,145\lambda$	$0.009\,853\,945\,311\,642\lambda$
500	$0.001\,992\,603\,359\,200\lambda$	$0.001\,992\,880\,765\,846\lambda$	$0.001\,993\,079\,888\,610\lambda$

N. Indeed, we have by means of (2.9) that

$$
E_{nl}^N = 2\beta(2n+\zeta) + \frac{\lambda\beta^\zeta\,\mathrm{e}^{\beta/g}}{g^{\zeta+1}\Gamma(\zeta)}\frac{(\zeta)_n}{n!}\sum_{i=0}^{n}\sum_{j=0}^{n}\frac{(-n)_i(-n)_j}{(\zeta)_i(\zeta)_j i!j!}
$$

$$
\times\left(\frac{\beta}{g}\right)^{i+j}\Gamma(\zeta+i+j+1)\Gamma\left(-\zeta-i-j;\frac{\beta}{g}\right) - \frac{A\beta}{\zeta-1}.
$$

In particular, if $A = 0$ and $B = 1$, we have

$$
E_{nl}^N = 4n + N + 2l + \frac{\lambda\,\mathrm{e}^{1/g}\left(\frac{N}{2}+l\right)_n}{n!g^{\frac{N}{2}+l+1}\Gamma\left(\frac{N}{2}+l\right)}\sum_{i=0}^{n}\sum_{j=0}^{n}\frac{(-n)_i(-n)_j g^{-i-j}}{\left(\frac{N}{2}+l\right)_i\left(\frac{N}{2}+l\right)_j i!j!}
$$

$$
\times\Gamma\left(\frac{N}{2}+l+i+j+1\right)\Gamma\left(-\frac{N}{2}-l-i-j;\frac{1}{g}\right).
$$

In table 5, we have expressed the first few states for different values of g and for small values of λ in the case of $N = 3$ and $l = 0$.

4. Conclusion

We have developed and applied a variational method to compute accurate upper bounds for the energies corresponding to the non-polynomial oscillator potential (1.1) in arbitrary dimension N. The results show the effectiveness of this approach in comparison with other techniques. We have compared our variational results with many other techniques developed in the literature, for example with the pseudo-perturbation expansion method [53], the shifted $1/N$ expansion [47], and the matrix continued fraction algorithm [49]. For each technique, we have confirmed their results with the use of very few matrix elements. Indeed, *all* of our variational bounds were obtained by the optimization of a square matrix (2.15) with size D not exceeding 20; these results can, of course, be further improved by simply increasing D.

Acknowledgments

Appendix. An infinite set of exact solutions

In this appendix, we investigate the exact solutions of the non-polynomial oscillator Schrödinger equation in the *N*-dimensional case. The existence of an infinite number of exact solutions of the one-dimensional Schrödinger equation (2.1) $(B = 1, N = 1, l = 0)$ with eigenfunctions given by products of exponential and polynomial functions of r^2, for specific relations between the couplings g and λ, was first reported by Flessas [22] and soon afterwards was extended by Varma [23]. The main point of exploring these exact solutions in this appendix is that: (1) they generalize the pervious exact solutions obtained for the one-dimensional case, and they are valid for arbitrary $\gamma = l + \frac{1}{2}(N - 3) \geqslant -1$; (2) they provide interesting examples for testing the validity and accuracy of our variational technique. Assuming

$$\psi(r) \equiv \phi_{nl}^N(r) = r^{\gamma+1} e^{-r^2/2} \sum_{i=0}^{n} \alpha_i r^{2i} \tag{A.1}$$

and substituting it into equation (2.1) yields $\left(B = 1, E \equiv E_{nl}^N\right)$

$$(E - 2\gamma - 3)\alpha_0 + (6 + 4\gamma)\alpha_1 + \sum_{i=1}^{n-1}\{(-2g(2i - 2) - \lambda + g(E - 2\gamma - 3))\alpha_{i-1} + (2ig(2i - 2)$$
$$- 4i + 4ig(\gamma + 1) + E - 2\gamma - 3)\alpha_i + (2(i + 1)(2i + 2\gamma + 3))\alpha_{i+1}\}r^{2i}$$
$$+ \{(-4g(n - 1) - \lambda + g(E - 2\gamma - 3))\alpha_{n-1} + (2ng(2n - 1)$$
$$- 4n + 4ng(\gamma + 1) + E - 2\gamma - 3)\alpha_n\}r^{2n}$$
$$+ (g(E - 2\gamma - 3) - \lambda - 4gn)a_n r^{2n+2} = 0.$$

The last term of this equation implies

$$\lambda = g(E - 4n - 2\gamma - 3), \qquad n = 0, 1, 2, \ldots \tag{A.2}$$

provided that the energy E and the interaction parameters λ, g satisfy the $(n + 1) \times (n + 1)$-tridiagonal determinant

$$\mathcal{D}_n(E) = \begin{vmatrix} b_0 & a_1 & 0 & 0 & \ldots & 0 & 0 & 0 \\ c_0 & b_1 & a_2 & 0 & \ldots & 0 & 0 & 0 \\ 0 & c_1 & b_2 & a_3 & \ldots & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & 0 & \ldots & c_{n-2} & b_{n-1} & a_n \\ 0 & 0 & 0 & 0 & \ldots & 0 & c_{n-1} & b_n \end{vmatrix} = 0, \tag{A.3a}$$

where

$$\begin{cases} a_n = g(E - 4n - 2\gamma - 3) - \lambda, \\ b_n = 2ng(2n + 2\gamma + 1) - 4n + E - 2\gamma - 3 = E - 4n - 2\gamma - 3 + gc_n, \\ c_n = 2n(2n + 2\gamma + 1), n = 0, 1, 2, \ldots. \end{cases} \tag{A.3b}$$

This determinantal equation can be written using the LU decomposition as

$$\mathcal{D}_n(E) = \begin{vmatrix} 1 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 \\ t_0 & 1 & 0 & 0 & \ldots & 0 & 0 & 0 \\ 0 & t_1 & 1 & 0 & \ldots & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & 0 & \ldots & t_{n-2} & 1 & 0 \\ 0 & 0 & 0 & 0 & \ldots & 0 & t_{n-1} & 1 \end{vmatrix}$$

$$\times \begin{vmatrix} u_0 & v_1 & 0 & 0 & \ldots & 0 & 0 & 0 \\ 0 & u_1 & v_2 & 0 & \ldots & 0 & 0 & 0 \\ 0 & 0 & u_2 & v_3 & \ldots & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & 0 & \ldots & 0 & u_{n-1} & v_n \\ 0 & 0 & 0 & 0 & \ldots & 0 & 0 & u_n \end{vmatrix}$$

in which

$$u_n = b_n - \frac{c_n a_{n-1}}{u_{n-1}}, \qquad u_0 = b_0, \qquad v_n = a_n, \qquad t_n = \frac{c_n}{u_{n-1}}.$$

This immediately leads to the following simple expression of computing the polynomial conditions as

$$\mathcal{D}_n(E) = \prod_{k=1}^{n} u_k = \prod_{k=1}^{n} \left(b_n - \frac{c_n a_{n-1}}{u_{n-1}} \right) = 0. \tag{A.4}$$

It should be clear that our relations (A.3)–(A.4) summarize the exact solutions not only in the N-space dimension where $\gamma = l + \frac{1}{2}(N - 3)$ but also for arbitrary real values of $\gamma \geqslant -1$.

References

[1] Biswas S N, Saxen R P, Srivastava P K and Varma V S 1973 *J. Math. Phys.* **14** 1190
[2] Salam A and Strathdee J 1970 *Phys. Rev.* D **1** 3296
[3] Risken H and Vollmer H D 1967 *Z. Phys.* **201** 323
[4] Haken H 1970 *Laser Theory (Encyclopedia of Physics* vol XXV/2c*)* (Princeton, NJ: Van Nostrand)
[5] Mitra A K 1978 *J. Math. Phys.* **19** 2018
[6] Kaushal S R 1979 *J. Phys. A: Math. Gen.* **12** L253
[7] Killingbeck J 1979 *Comput. Phys. Commun.* **18** 211
[8] Galicia S and Killingbeck J 1979 *Phys. Lett.* A **71** 17
[9] Bessis N and Bessis G 1980 *J. Math. Phys.* **21** 2780
[10] Hautot A 1981 *J. Comput. Phys.* **39** 72
[11] Lai C S and Lin H E 1982 *J. Phys. A: Math. Gen.* **15** 1495
[12] Witwit M R M 1994 *Indian J. Pure Appl. Phys.* **32** 391
[13] Bessis N, Bessis G and Hadinger G 1983 *J. Phys. A: Math. Gen.* **16** 497
[14] Cohen M 1984 *J. Phys. A: Math. Gen.* **17** 2345
[15] Fack V and Vanden Berghe G 1985 *J. Phys. A: Math. Gen.* **18** 3355
[16] Fack V and Vanden Berghe G 1986 *Comp. Phys. Commun.* **39** 187
[17] Fack V, De Meyer H and Vanden Berghe G 1986 *J. Math. Phys.* **27** 1340
[18] Fack V and Vanden Berghe G 1987 *J. Phys. A: Math. Gen.* **20** 4153
[19] Handy C R 1985 *J. Phys. A: Math. Gen.* **18** 2141
[20] Hodgson R J W 1988 *J. Phys. A: Math. Gen.* **21** 1563
[21] Agrawal R K and Varma V S 1993 *Phys. Rev.* A **48** 1921
[22] Flessas G P 1981 *Phys. Lett.* A **83** 121
[23] Varma V S 1981 *J. Phys. A: Math. Gen.* **14** L489
[24] Whitehead R P, Watt A, Flessas G P and Nagarajan M A 1982 *J. Phys. A: Math. Gen.* **15** 1217
[25] Heading J 1982 *J. Phys. A: Math. Gen.* **15** 2355
[26] Heading J 1983 *J. Phys. A: Math. Gen.* **16** 2121
[27] Flessas G P 1982 *J. Phys. A: Math. Gen.* **15** L97
[28] Chaudhuri R N and Mukherjee B 1983 *J. Phys. A: Math. Gen.* **16** 4031
[29] Marcilhacy G and Pons R 1985 *J. Phys. A: Math. Gen.* **18** 2441
[30] Marcilhacy G and Pons R 1991 *Phys. Lett.* A **152** 235
[31] Blecher M H and Leach P G 1987 *J. Phys. A: Math. Gen.* **20** 5927
[32] Gallas J A C 1988 *J. Phys. A: Math. Gen.* **21** 3393
[33] Roy P and Roychoudhury R 1987 *Phys. Lett.* A **122** 275
[34] Roy P, Roychoudhury R and Varshni Y P 1988 *J. Phys. A: Math. Gen.* **21** 1589
[35] Vanden Berghe G and De Meyer H E 1989 *J. Phys. A: Math. Gen.* **22** 1705

[36] Lakhtakia A 1989 *J. Phys. A: Math. Gen.* **22** 1701
[37] Roy P and Roychoudhury R 1990 *J. Phys. A: Math. Gen.* **23** 1657
[38] Fernandez F M 1991 *Phys. Lett.* A **160** 116
[39] Bose S K and Varma N 1989 *Phys. Lett.* A **141** 141
[40] Hislop D, Wolfaardt M F and Leach P G L 1990 *J. Phys. A: Math. Gen.* **23** L1109
[41] Stubbins C and Gornstein M 1995 *Phys. Lett.* A **202** 34
[42] Hall R L and Zhou Wei Hua 1998 *Can. J. Phys.* **76** 31
[43] Ishikawa H 2002 *J. Phys. A: Math. Gen.* **35** 4453
[44] Handy C R, Hay H, Stephens D V, Joshua J and Summerour S 1993 *J. Phys. A: Math. Gen.* **26** 2649
[45] Znojil M 1983 *J. Phys. A: Math. Gen.* **16** 279
[46] Znojil M 1984 *J. Phys. A: Math. Gen.* **17** 3441
[47] Varshni Y P 1987 *Phys. Rev.* A **36** 3009
[48] Roy B, Roychoudhury R and Roy P 1988 *J. Phys. A: Math. Gen.* **21** 1579
[49] Scherrer H, Risken H and Leiber T 1988 *Phys. Rev.* A **38** 3949
[50] Adhikari R, Dutt R and Varshni 1991 *J. Math. Phys.* **32** 447
[51] Witwit M R M 1991 *J. Phys. A: Math. Gen.* **24** 5291
[52] Witwit M R M 1996 *J. Comput. Phys.* **129** 220
[53] Mustafa O and Odeh M 2001 Conference on Analysis and Mathematical Physics (Lund University) *Preprint* math-ph/0101029
[54] Hall L R, Saad N and Keviczky A B 2002 *J. Math. Phys.* **43** 94
[55] Ferreira C, López J L and Sinusa E P 2005 *Adv. Appl. Math.* **34** 467
[56] Temme M N 1996 *Special Functions* (New York: Wiley-Interscience) chapter 11, formula 11.7
[57] Chen H 1998 The quadrature discretization method and its applications *PhD Thesis* University of British Columbia
[58] Chen H and Shizgal B D 1998 *J. Math. Chem.* **24** 321
[59] Imbo T, Pagnamenta A and Sukhatme U 1984 *Phys. Rev. D* **29** 1669