Certain class of generalized isotropic perturbations of the s-wave three-dimensional harmonic oscillator

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Abstract. In this paper we study a certain class of generalized perturbation problem for the isotropic three dimensional harmonic oscillator, for $l = 0$ states only, for all excited states. The efficacy of our formalism is tested by studying the Killingbeck potential in detail. We also briefly present our results using the diagonal Padé approximants.

Keywords. Perturbation theory; Padé approximants; Killingbeck potential; three-dimensional harmonic oscillator.

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1. Introduction

In the present work we have investigated the most general perturbation of a three-dimensional harmonic oscillator (for $l = 0$ states only). Such a perturbation can be written as,

$$V(r) = \beta \sum_{i=0}^{\infty} {}' b_i r^{i-1},\tag{1}$$

where the prime indicates that the $i = 3$ term (i.e. the harmonic oscillator potential term) is not present because it forms a part of the unperturbed Hamiltonian. A similar potential was investigated by Iafrate and Mandelsohn (1970) regarding it as a perturbation to the Coulomb potential. Further, since we are dealing with $l = 0$ states only, terms corresponding to $i \leqslant -1$ in (1) would render such a system unstable. Such potentials have been found useful in describing the dynamics of quark-quark and quark-antiquark systems (Quigg and Rosner 1979; Grosse and Martin 1980) and complex atoms with screened Coulomb potentials (Bednar 1973).

Recently, Killingbeck (1978) studied a special case of such a potential:

$$V(r) = -1/r + 2\lambda r + 2\lambda^2 r^2,\tag{2}$$

which possesses an exact ground state $E = 3\lambda - 1/2$ for $\lambda \geqslant 0$. However, the energy spectrum of this system possesses a singularity at $\lambda = 0$. In fact, it was shown by Saxena and Varma (1982) that the correct expansion parameter for a Rayleigh Schrödinger (RS) perturbation series of energy is $|\lambda|^{-1/2}$ and not λ. In this paper, we have investigated the perturbation problem for the potential given by equation (1) to all orders of perturbation for the ground state and all the excited states. As an illustration

of the general formalism, we have discussed the ground state and four of the excited states for the Killingbeck potential (equation (2)), in detail. Since it is well known that the RS series is asymptotic in nature (Dyson 1952), we have computed Padé approximants to get rapidly converging answers for the energy eigenvalues.

In §2 we outline our perturbation formalism. In §3 we apply the formalism to the Killingbeck potential for both attractive and repulsive Coulomb terms and convert the resulting RS series into Padé approximants. A brief discussion of our results as compared to the precise Hill determinant results is also given.

2. Perturbation formalism

The complete radial Schrödinger equation for our system with the perturbing potential of the form (1) is,

$$
\left(-\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{1}{2}w^2r^2 + \beta \sum_{i=0}^{\infty}{}' b_i r^{i-1} \right)
$$

$$
\times \phi^{(m)}(r) = E^{(m)}\phi^{(m)}(r), \tag{3}
$$

where $E^{(m)}$ and $\phi^{(m)}$ are the mth excited state and the corresponding radial eigenfunction. We now expand the wavefunction and energy in terms of the perturbation parameter β as,

$$
\phi^{(m)} = \sum_{j=0}^{\infty} \phi_j^{(m)}\beta^j \tag{4a}
$$

and

$$
E^{(m)} = \sum_{p=0}^{\infty} E_p^{(m)}\beta^p. \tag{4b}
$$

Substituting (4) in (3) and equating the coefficients of β^k on both sides, we obtain,

$$
\left(-\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{1}{2}w^2r^2 \right)\phi_k^{(m)}(r) + \sum_{i=0}^{\infty}{}' b_i r^{i-1} \phi_{k-1}^{(m)}(r)
$$

$$
= \sum_{q=0}^{k} E_{k-q}^{(m)}\phi_q^{(m)}(r). \tag{5}
$$

We look for a solution of the form

$$
\phi_k^{(m)}(r) = r^t \exp(-wr^2/2)u_k^{(m)}(r). \tag{6}
$$

With the choice $t = -1$, we recognise $u_0^{(m)}(r)$ as,

$$
u_0^{(m)}(r) = N_m H_{2m+1}(\sqrt{w}r), \tag{7a}
$$

where $m = 0, 1, 2,\ldots$. Here $H_{2m+1}(\sqrt{w}r)$ are Hermite polynomials and N_m is the normalization constant. The zeroth order energy will be given by,

$$
E_0^{(m)} = (1/2)(4m + 3)w. \tag{7b}
$$

We now expand the higher order reduced radial wave functions $u_k^{(m)}$ in terms of Hermite polynomials as,

$$u_k^{(m)}(r) = \sum_{n=0}^{\infty} A_{k,n}^{(m)} N_n H_{2n+1}(\sqrt{w}\,r),$$ (8)

where obviously,

$$A_{0,n}^{(m)} = \delta_{nm}.$$ (8a)

Using simple properties of Hermite polynomials (Mathews and Venkatesan 1976) equation (5) becomes,

$$2w(m-1)A_{k,l}^{(m)} + E_k^{(m)}\delta_{lm}$$

$$= \sum_{n=0}^{\infty} A_{k-1,n}^{(m)} \sum_{i=0}^{\infty}{}' b_i I(n, l, i-1) - \sum_{q=1}^{k-1} E_{k-q}^{(m)} A_{q,l}^{(m)},$$ (9)

where $I(n, l, \alpha)$ are given by,

$$I(n, l, \alpha) = N_n N_l \int [\exp(-wr^2)/r^2] H_{2n+1}(\sqrt{w}\,r) H_{2l+1}(\sqrt{w}\,r) r^\alpha d^3 r$$

$$= \frac{(-1)^{n+1}}{2w^{(i-1/2)}} \left(\frac{\Gamma(n+1)\Gamma(l+1)}{\Gamma(n+3/2)\Gamma(l+3/2)} \right)^{1/2}$$

$$\times \sum_{s=0}^{n \text{ or } l} \frac{\Gamma(3/2 + \alpha/2 + s)\Gamma(n - \alpha/2 - s)\Gamma(l - \alpha/2 - s)}{\Gamma^2(-\alpha/2)\Gamma(s+1)\Gamma(n-s+1)\Gamma(l-s+1)}.$$ (10)

Some details about the evaluation of these integrals are given in the Appendix.

Equation (9) forms the basis of our perturbation calculation. A look at the structure of this equation tells us that for $l = m$, it yields the kth order contribution to the mth excited state energy ($E_k^{(m)}$), while for $l \neq m$ all the coefficients of the wavefunction ($A_{k,l}^{(m)}$) are obtained. These equations are:

$$E_k^{(m)} = \sum_{n=0}^{\infty} A_{k-1,n}^{(m)} K(n, m) - \sum_{q=1}^{k-1} E_{k-q}^{(m)} A_{q,m}^{(m)},$$ (11)

$$A_{k,l}^{(m)} = (1/(2(m-l)w)) \left[\sum_{n=0}^{\infty} A_{k-1,n}^{(m)} K(n, l) - \sum_{q=1}^{k-1} E_{k-q}^{(m)} A_{q,l}^{(m)} \right]$$ (12)

where

$$K(n, m) = \sum_{i=0}^{\infty}{}' b_i I(n, m, i-1).$$ (13)

$A_{k,m}^{(m)}$'s are evaluated demanding that the wavefunction be normalized to the kth order, and are found to be,

$$A_{k,m}^{(m)} = -\sum_{j=1}^{k-1} \beta^{j-k} A_{j,m}^{(m)} - (1/2) \sum_{n=0}^{\infty} \sum_{j=1}^{k-1} \sum_{j'=1}^{k-1} A_{j,n}^{(m)} A_{j',n}^{(m)} \beta^{j+j'-k},$$ (14)

here j and j' take on integral values such that $j + j' - k \leqslant 0$ is always satisfied. We list below a few coefficients of the energy expansion:

$$E_0^{(m)} = \tfrac{1}{2}(4m + 3)w,$$

$$E_1^{(m)} = K(m, m),$$

$$E_2^{(m)} = \sum_{n=0}^{\infty}{}' \frac{K^2(n, m)}{2(m - n)w},$$

$$E_3^{(m)} = \sum_{n=0}^{\infty}{}' \frac{K(n, m)}{4w(m - n)} \left[\sum_{j=0}^{\infty}{}' \frac{K(j, m)K(j, n)}{(m - j)} - \frac{K(m, m)K(m, n)}{(m - n)} \right]. \tag{15}$$

Some low order wavefunction coefficients are:

$$A_{0,n}^{(m)} = \delta_{nm},$$

$$A_{1,l}^{(m)} = \frac{K(m, l)}{2(m - l)w} \quad \text{(for } l \neq m)$$

$$A_{1,m}^{(m)} = 0$$

$$A_{2,l}^{(m)} = (1/(2(m - l)w)) \left[\sum_{n=0}^{\infty}{}' \frac{K(n, m)K(n, l)}{2(m - n)w} - \frac{K(m, m)K(m, l)}{2(m - l)w} \right],$$

$$\text{(for } l \neq m)$$

$$A_{2,m}^{(m)} = (-1/8) \sum_{n=0}^{\infty}{}' \frac{K^2(n, m)}{(m - n)^2 w^2}, \tag{16}$$

where the prime on the summations implies $m \neq n$ and $j \neq m$.

Equations (11) and (12) yield, in principle, all energy eigenvalues and eigenfunctions to all orders of perturbation.

3. Discussion

As an illustration of the formalism developed in the previous section, we discuss a generalization of the potential considered by Killingbeck (1978) and Saxena and Varma (1982). The radial Schrödinger equation for this potential ($l = 0$ states) is given by,

$$\left(-\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + V(r) \right) \psi^{(m)}(r) = E^{(m)} \psi^{(m)}(r), \tag{17}$$

where

$$V(r) = \pm 1/r + 2\lambda r + 2\lambda^2 r^2. \tag{18}$$

The $\pm$ signs for the $1/r$ term in the potential denote the repulsive (attractive) nature of the Coulomb force and the other terms denote the polynomial perturbation. In (17), $\psi^{(m)}(r)$ and $E^{(m)}$ are the energy eigenfunction and eigenvalue respectively of the mth excited state.

By a simple coordinate transformation $z = (|\lambda|)^{1/2} r$ (17) can be rewritten as,

$$\left[-\frac{1}{2}\frac{d^2}{dz^2} - \frac{1}{z}\frac{d}{dz} + 2r^2 + (1/\sqrt{|\lambda|})(2(\lambda/|\lambda|)z \mp 1/z) \right]\phi^{(m)}(z)$$

$$= \mathscr{E}^{(m)}\phi^{(m)}(z) \tag{19}$$

where

$$\mathscr{E}^{(m)} = E^{(m)}/|\lambda|, \quad \phi^{(m)}(z) = \psi^{(m)}(r). \tag{19a}$$

It is easy to see that by choosing $w = 2, b_0 = \mp 1, b_2 = 2(\lambda/|\lambda|)$ and all other b_i's equal to zero, (19) becomes a special case of (3). We now utilize equations (11) and (12) to evaluate the ground state as well as four excited state energies and their corresponding wavefunction up to 40th orders of perturbation. For the perturbation given by (18), (13) simplifies to,

$$K(n, m) = \frac{(-1)^{(m+n)}}{\sqrt{2}}\left(\frac{\Gamma(m+1)\Gamma(n+1)}{\Gamma(m+3/2)\Gamma(n+3/2)}\right)^{1/2}\sum_{s=0}^{m\ or\ n}\frac{\Gamma(m-s-1/2)}{\Gamma(m-s+1)}$$

$$\times \frac{\Gamma(n-s-1/2)}{\Gamma(n-s+1)}[(\lambda/|\lambda|)((s+1)/4)$$

$$\mp (m-s-1/2)(n-s-1/2)]. \tag{20}$$

The unperturbed energy ($\mathscr{E}_0^{(m)}$) and the first order shifts in energy ($\mathscr{E}_1^{(m)}$) are known exactly. Also, it is found that the energy coefficients $\mathscr{E}_2^{(m)}$ and $\mathscr{E}_3^{(m)}$ are independent of λ, the coupling constant. Further, in the evaluation of $\mathscr{E}_2^{(m)}$, a single slowly converging series is involved. The number of terms required to obtain a sum of this series correct to twelve significant figures is of the order of 50,000. However, $\mathscr{E}_3^{(m)}$ involves a double summation and thus to evaluate $\mathscr{E}_3^{(m)}$ to the same degree of precision as $\mathscr{E}_2^{(m)}$ requires numerical work of a prohibitive order of magnitude. Thus for evaluation of $\mathscr{E}_3^{(m)}$ and other higher order perturbation energies we adopt a $100 \otimes 100$ matrix approximation in equations (11) and (12). We shall attempt no further justification of this approximation except *a posteriori*, when we compare our results with those obtained by the Hill determinant method.

Table 1. Progressive convergence of diagonal Padé approximants of the perturbation series for the first excited state (E_1) for $\lambda = -0.08$ in the case of repulsive Coulomb interaction.

$P(1, 1)$	$0.56000000(+0)$	$P(11, 11)$	$-0.77271659(-1)$
$P(2, 2)$	$-0.25842557(+1)$	$P(12, 12)$	$-0.77229730(-1)$
$P(3, 3)$	$-0.85027423(-1)$	$P(13, 13)$	$-0.77325926(-1)$
$P(4, 4)$	$-0.81384093(-1)$	$P(14, 14)$	$-0.77311461(-1)$
$P(5, 5)$	$-0.76928609(-1)$	$P(15, 15)$	$-0.77277607(-1)$
$P(6, 6)$	$-0.76282437(-1)$	$P(16, 16)$	$-0.77312069(-1)$
$P(7, 7)$	$-0.76218981(-1)$	$P(17, 17)$	$-0.77310130(-1)$
$P(8, 8)$	$-0.76201381(-1)$	$P(18, 18)$	$-0.77309875(-1)$
$P(9, 9)$	$-0.76397190(-1)$	$P(19, 19)$	$-0.77312429(-1)$
$P(10, 10)$	$-0.76394128(-1)$	$P(20, 20)$	$-0.77311210(-1)$

It is well known that the RS perturbation series for the energy eigenvalues is only an asymptotic expansion in powers of the coupling constant (Dyson 1952). To estimate the sum of such a series, several methods are known in the mathematical literature (Whittaker and Watson 1962; Simon 1970). In this paper we have chosen to estimate the sum of the RS series by a sequence of diagonal Padé approximants $P(m, m)$. It is well known through the pioneering work of Padé, Hadamard, Stieltjes and Borel that for a class of series of Stieltjes (Baker and Gammel 1970) the Padé approximants provide a convergent sum on a cut plane with a finite radius of convergence. The asymptotic perturbation theory in our case, hopefully provides an example of such a convergence. The numerical computations displayed in table 1 bear this out. In tables 2 and 3 we list the ground state and the first four excited states for the potentials $-1/r + 2\lambda r + 2\lambda^2 r^2$ and $1/r + 2\lambda r + 2\lambda^2 r^2$ for positive as well as negative λ (for $|\lambda| = 8\cdot0$, $0\cdot8$, $0\cdot08$). Our results are also compared with the Hill determinant results of Saxena et al (1987). It can be clearly seen that for larger values (since our expansion parameter is $|\lambda|^{-1/2}$) our results are in good agreement with the precise Hill determinant results. However as $|\lambda| < 0\cdot1$ this agreement slowly deteriorates, as is to be expected. For $|\lambda| > 1$ our

Table 2a*. Energy levels of the Killingbeck potential with attractive Coulomb interaction for $|\lambda| = 8\cdot0$.

Energy** eigenvalues	Coupling constant = $+8\cdot0$	Coupling constant = $-8\cdot0$
E_0	0·2350007 (+2)	0·1494122 (+2)
	0·23500000(+2)	0·14941198(+2)
E_1	0·5874234 (+2)	0·4541873 (+2)
	0·58742278(+2)	0·45418716(+2)
E_2	0·9291586 (+2)	0·7613010 ̇(+2)
	0·92915803(+2)	0·76130078(+2)
E_3	0·12663380(+3)	0·10699014(+3)
	0·12663373(+3)	0·10699011(+3)
E_4	0·16008935(+3)	0·13795574(+3)
	0·16008929(+3)	0·13795572(+3)

*The figures in brackets against every entry in tables 2a to 3c represent the exponent to the base ten.

**The first row against each E_n in tables 2a to 3c displays the eigenvalues calculated from summation of the perturbation series by Padé approximants whereas the next row gives the corresponding eigenvalues calculated by Hill determinant (HD) method. It should be noted that the eigenvalues calculated by HD method are known to converge up to 16 significant figures or more, however the lesser number of digits are quoted here only for a comparison with the values calculated by perturbation method.

Table 2b. Energy levels of the Killingbeck potential with attractive Coulomb interaction for $|\lambda| = 0.8$.

Energy eigenvalues	Coupling constant = + 0·8	Coupling constant = − 0·8
E_0	0·19004 (+ 1)	− 0·49045 (+ 0)
	0·19000000 (+ 1)	− 0·49055768(+ 0)
E_1	0·62958 (+ 1)	0·221629 (+ 1)
	0·62954761 (+ 1)	0·22161983 (+ 1)
E_2	0·102261 (+ 2)	0·500243 (+ 1)
	0·10225765 (+ 2)	0·50023400 (+ 1)
E_3	0·139884 (+ 2)	0·783798 (+ 1)
	0·13988135 (+ 2)	0.78378892 (+ 1)
E_4	0·176595 (+ 2)	0·1070817 (+ 2)
	0·17659107 (+ 2)	0·10708074 (+ 2)

Table 2c. Energy levels of the Killingbeck potential with attractive Coulomb interaction for $|\lambda| = 0.08$.

Energy eigenvalues	Coupling constant = + 0·08	Coupling constant = − 0·08
E_0	− 0·2560 (+ 0)	− 0·7244 (+ 0)
	− 0·26000000 (+ 0)	− 0·72578783 (+ 0)
E_1	0·6331 (+ 0)	− 0·5612 (+ 0)
	0·63123363 (+ 0)	− 0·56151836 (+ 0)
E_2	0·1221 (+ 1)	− 0·3755 (+ 0)
	0·12193701 (+ 1)	− 0·37591029 (+ 0)
E_3	0·1734 (+ 1)	− 0·1733 (+ 0)
	0·17325956 (+ 1)	− 0·17381198 (+ 0)
E_4	0·2211 (+ 1)	0·406 (− 1)
	0·22098669 (+ 1)	0·40081514 (− 1)

perturbation series itself gives a rapidly converging result, in excellent agreement with Hill determinant results.

Table 3a. Energy levels of the Killingbeck potential with repulsive Coulomb interaction for $|\lambda| = 8\cdot0$.

Energy eigenvalues	Coupling constant $= +8\cdot0$	Coupling constant $= -8\cdot0$
E_0	0·3299828 (+2)	0·2349996 (+2)
	0·32998295(+2)	0·23500000(+2)
E_1	0·6648478 (+2)	0·5271319 (+2)
	0·66484797(+2)	0·52713234(+2)
E_2	0·9975362 (+2)	0·8267719 (+2)
	0·99753638(+2)	0·82677240(+2)
E_3	0·13288097(+3)	0·11302278(+3)
	0·13288099(+3)	0·11302284(+3)
E_4	0·16590658(+3)	0·14360313(+3)
	0·16590661(+3)	0·14360318(+3)

Table 3b. Energy levels of the Killingbeck potential with repulsive coulomb interaction for $|\lambda| = 0\cdot8$.

Energy eigenvalues	Coupling constant $= +0\cdot8$	Coupling constant $= -0\cdot8$
E_0	0·522846 (+1)	0·189994 (+1)
	0·52284979(+1)	0·19000000(+1)
E_1	0·888643 (+1)	0·435753 (+1)
	0·88864840(+1)	0·43575936(+1)
E_2	0·1248077 (+2)	0·696525 (+1)
	0·12480817(+2)	0·69653078(+1)
E_3	0·1603275 (+2)	0·966712 (+1)
	0·16032798(+2)	0·96671627(+1)
E_4	0·1955388 (+2)	0·1243252 (+2)
	0·19553923(+2)	0·12432547(+2)

Table 3c. Energy levels of the Killingbeck potential with repulsive Coulomb interaction for $|\lambda| = 0.08$.

Energy eigenvalues	Coupling constant $= +0.08$	Coupling constant $= -0.08$
E_0	0·112225 $(+1)$	$-0·259999$ $(+0)$
	0·11223013$(+1)$	$-0·26000000(+0)$
E_1	0·157623 $(+1)$	$-0·7731$ (-1)
	0·15763096$(+1)$	$-0·77311245(-1)$
E_2	0·201423 $(+1)$	0·111 $(+0)$
	0·20143126$(+1)$	0·11177777$(+0)$
E_3	0·24409 $(+1)$	0·307 $(+0)$
	0·24410103$(+1)$	0·30807994$(+0)$
E_4	0·285913 $(+1)$	0·51 $(+0)$
	0·28591670$(+1)$	0·51182116$(+0)$

Appendix

We need to evaluate integrals of the type:

$$J(n,l,\alpha) = \int_0^\infty \exp(-v^2)v^\alpha H_{2n+1}(v)H_{2l+1}(v)\,dv. \tag{A1}$$

We use the well-known relation between Hermite polynomials and the confluent hypergeometric (CH) functions (Abromowitz and Stegun 1972) and a contour integral representation for the resulting CH function $(F(-1,3/2,t))$(Landau and Lifshitz 1958). The original integral now looks like the Laplace transform of a single CH function (Landau and Lifshitz 1958) and can now be evaluated to give:

$$J(n,l,\alpha) = \frac{(-1)^{n+l+1}}{4i} \frac{(2n+1)!(2l+1)!}{\Gamma(n+3/2)\Gamma(l+3/2)}$$

$$\times \sum_{r=0}^{l} \frac{\Gamma(3/2+\alpha/2+r)\Gamma(l-r-\alpha/2)}{\Gamma(-\alpha/2)\Gamma(r+1)\Gamma(m-r+1)}$$

$$\times \oint (-z)^{-n-1+r}(1-z)^{n-\alpha/2-r-1}\,dz. \tag{A2}$$

The remaining contour integral in (A2) can be recognised to be an integral representation of the hypergeometric function (Landau and Lifshitz 1958). The final result after some simplification of the hypergeometric function yields:

$$J(n,l,\alpha) = (-1)^{n+1}\frac{\pi}{2}\frac{(2n+1)!(2l+1)!}{\Gamma(n+3/2)\Gamma(l+3/2)}$$

$$\times \sum_{r=0}^{l} \frac{\Gamma(3/2+\alpha/2+r)\Gamma(n-r-\alpha/2)\Gamma(l-r-\alpha/2)}{\Gamma^2(-\alpha/2)\Gamma(r+1)\Gamma(n-r+1)\Gamma(l-r+1)}. \tag{A3}$$

Acknowledgements

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