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ADDENDUM

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Abstract. Ground and excited state energy levels of the Schrödinger equation for various model potentials in two-dimensional space are calculated, using inner product and renormalized series techniques, over wide ranges of relevant perturbation parameters. Mixed parity potentials are treated, whereas earlier works have treated only even parity perturbations.

This work describes a generalization to the case of mixed parity perturbations of the inner product perturbation theory for the two-dimensional perturbed oscillator. The basic theory of the method has been reported earlier for the case of even parity perturbations [1, 2]. We take the Schrödinger equation in the form

$$\left[-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+x^2+y^2+\lambda V(x,y)\right]\Psi(x,y)=E\Psi(x,y) \tag{1}$$

and the perturbing potential in the non-separable form

$$V(x,y)=[a_{xx}x^4+4b_{xy}x^3y+6c_{xy}x^2y^2+4b_{yx}xy^3+a_{yy}y^4] \tag{2}$$

which we re-write to include a renormalization parameter α:

$$V^r(x,y)=\beta^2[x^2+y^2]+\lambda[V(x,y)-\alpha(x^2+y^2)] \tag{3}$$

with

$$\beta^2=1+\lambda\alpha. \tag{4}$$

Varying α improves the convergence properties of the energy perturbation series and enables numerical results to be obtained for many energy levels and over a wide range of λ values.

The principal recurrence relation is obtained by introducing the reference function:

$$\Phi(x,y)=(x^{n_x}y^{n_y})\exp\left[-\frac{\beta}{2}(x^2+y^2)\right] \tag{5}$$

where n_x and n_y are state numbers, with values, 0, 1, 2, ... To determine the energy eigenvalue, we begin from the equation

$$ER(M,N)=\langle\Psi|Hx^My^N|\Phi\rangle \tag{6}$$

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Table 1. Eigenvalues of $E^{\pi}_{n_x,n_y}$ for several eigenstates for the potential (3) using the inner product technique for several sets of perturbation parameters. The parity label ($\pi = +, -$; even, odd) for the $x \leftrightarrow y$ interchange symmetry.

E^{+}_{00}					
λ	$a_{xx}=b_{xy}=c_{xy}=b_{yx}=a_{yy}=1$	$a_{xx}=c_{xy}=a_{yy}=1$, $b_{xy}=b_{yx}=0$	$a_{xx}=a_{yy}=0$, $c_{xy}=b_{xy}=b_{yx}=1$	$a_{xx}=c_{xy}=a_{yy}=1$ $b_{xy}=b_{yx}=-1$	$c_{xy}=1, a_{xx}=b_{xy}=b_{yx}=a_{yy}=0$
0.001	2.00297932550	2.002989582298	2.00148629485	2.00297932550	2.0014966434
0.005	2.01451240904	2.014747344162	2.00717284290	2.01451240904	2.0074178539
0.01	2.02817285463	2.029024818098	2.01375771519	2.02817285463	2.0146796702
0.02	2.05346792878	2.056345709271	2.02545748502	2.05346792878	2.0287781095
0.03	2.07663858468	2.082246879492	2.03552521	2.07663858468	2.0423683323
0.04	2.09814393728	2.106935857573	2.04422238	2.09814393728	2.0555076010
0.05	2.11829265436	2.130571019087	2.0517181	2.11829265436	2.0682421307
0.06	2.1373057146	2.153277169379	2.058120	2.1373057146	2.0806100458
0.07	2.155348501	2.175155111414	2.063486	2.155348501	2.0926433484
0.08	2.172548979	2.196287874566	2.06782	2.172548979	2.1043692859
0.09	2.189008781	2.216744955278	2.0711	2.189008781	2.1158113350
0.10	2.204810333	2.236585308734	2.0733	2.204810333	2.1269899290
0.11	2.22002164	2.255859521657	2.075	2.22002164	2.1379230082
0.12	2.2346997	2.274611429174	2.08	2.2346997	2.1486264441
0.13	2.2488927	2.292879343046		2.2488927	2.1591143729
0.14	2.2626421	2.310697001422		2.2626421	2.1693994602
0.15	2.2759836	2.328094314707		2.2759836	2.1794931149
0.20	2.337545	2.409620654744		2.337545	2.2274208365
0.25	2.392352	2.483708119302		2.392352	2.2717872084
0.50	2.6077	2.784703283061		2.6077	2.45837692
0.75	2.7697	3.018831386575		2.7697	2.608944
1.0	2.9035	3.215082605		2.9035	2.737919

λ	$a_{xx}=c_{xy}=a_{yy}=1$, $b_{xy}=b_{yx}=0$				
	E^{+}_{00}	E^{+}_{01}	E^{+}_{11}	E^{+}_{02}	E^{-}_{20}
0.01	2.02902481809	4.085808965642	6.19620400143	6.19620400143	6.1425931132
0.1	2.23658530873	4.657297942265	7.39554127136	7.39554127136	7.0781057579
1.0	3.21508260493	7.083325838485	11.9661246777	11.9661246777	10.951569072
10	6.01988963109	13.6531613279	23.7040560004	23.7040560004	21.286433025
100	12.5255366597	28.6372768319	50.0765646278	50.0765646278	44.749017003
1000	26.7768834021	61.332853812	107.423119169	107.423119169	95.888824225
5000	45.7232177421	104.76492582	183.547521435	183.547521435	163.80663391
10000	57.5919813668	131.96819737	231.220622305	231.220622305	206.34441333
100000	124.033083542	284.23818307	498.0496861	498.0496861	444.443284
10^6	267.2002505	612.33609	1072.960813	1072.690813	957.471918

λ	$a_{xx}=c_{xy}=a_{yy}=1$, $b_{xy}=b_{yx}=0$			$a_{xx}=\frac{1}{2}, a_{yy}=\frac{1}{4}, c_{xy}=1, b_{xy}=b_{yx}=0$	
	E^{+}_{31}	E^{-}_{13}	E^{+}_{22}	E^{+}_{01}	E^{-}_{10}
0.01	10.5643386463	10.41348644104	10.4979586107	4.06316187217	4.0559240197
0.1	13.5588944543	12.79677090567	13.2339429621	4.50378544338	4.4461010151
1.0	23.534707491	21.36059250479	22.6363423276	6.518873405	6.2540643
10	47.82744739	42.82351025463	45.7837545476	12.23496925	11.500257
100	101.6771803	90.73955672637	97.2229710547	25.47066894	23.786814
1000	218.420756	194.782639802	208.800621011	54.45693078	50.77898
5000	373.297505	332.85406087	356.839938301	92.9905411	86.68563
10000	470.277704	419.31662169	449.54068391	117.129344	109.1818
100000	1013.04535	903.23713867	968.3636937	252.25716	235.1238
10^6	2182.4756	1945.8942661	2086.21026	543.4282	506.509

obtained by taking the inner product of the Schrödinger equation (1) with the reference function (5). The $R(M, N)$, sometimes called moments, are defined by

$$R(M, N) = \langle \Psi | x^M y^N | \Phi \rangle. \tag{7}$$

Substituting the perturbation expansions

$$R(M, N) = \sum_K R(M, N, K)\lambda^K \tag{8}$$

$$E = \sum_J E(J)\lambda^J \tag{9}$$

into the $R(M, N)$ recurrence relations arising from equation (6) leads to a recurrence relation for the perturbation coefficients which is a generalization of that given previously [1,2];

$$\begin{aligned}\sum_{J=0}^{K} E(J)R(M, N, K-J) = {} & a_{xx}R(M+4, N, K-1) + a_{yy}R(M, N+4, K-1) \\ & + 6c_{xy}R(M+2, N+2, K-1) + 4b_{xy}R(M+1, N+3, K-1) \\ & + 4b_{yx}R(M+1, N+3, K-1) - \alpha[R(M+2, N, K-1) + R(M, N+2, K-1)] \\ & \times \beta[4M+4N+2n_x+2n_y+2]R(M, N, K) - M[2M+2n_x-1]R(M-2, N, K) \\ & - N[2N+2n_y-1]R(M, N-2, K).\end{aligned} \tag{10}$$

The unperturbed energy can be written in the form

$$E(0) = \beta[4S_x + 4S_y + 2n_x + 2n_y + 2] \tag{11}$$

where the indices S_x and S_y can be used to pick out particular states by using the initial condition $R(S_x, S_y, 0) = 1$. In general the indices M, N, K are scanned as explained in [1,2], and the various $R(M, N, K)$ are calculated recursively. For the special case $M = S_x$, $N = S_y$ the recurrence relation permits extraction of the energy coefficients $E(K)$, because of the condition $R(S_x, S_y, K) = \delta(0, K)$ which is imposed on the algorithm.

In the case of an isotropic perturbation V (i.e. for special choices of the potential coefficients) the hypervirial perturbation method [2] is applicable to the problem; we have checked that it then gives results in agreement with those of the inner product perturbation approach. For these special isotropic cases the potential can be expressed in a radial form

$$V(r) = \mu r^2 + [m^2 - \tfrac{1}{4}]r^{-2} + \lambda[r^4 - \alpha r^2] \tag{12}$$

where $\mu = 1 + \lambda\alpha$, α is the adjustable renormalization parameter and m is the magnetic quantum number. For both the inner product and hypervirial methods varying parameter α was found to be very effective in producing accurate numerical results from the perturbation series. Table 1 shows some typical results. Results for many more states and λ values are available from the authors and are deposited with the British Library Supplementary Publications Scheme, document no SUP 70048. We performed special internal checking calculations for the case $a_{xx} = a_{yy} = \frac{1}{3}$, $a_{xy} = \frac{1}{9}$, for which the perturbation can be written in the alternative form

$$V(x, y) = \lambda[x^4 + y^4] + 2\lambda^2 x^2 y^2 \tag{13}$$

with $\lambda = 1/3$. This form leads to an inner product perturbation calculation with λ and λ^2 terms, so that the terms of various orders of λ become differently mixed together in the energy series. The fact that this alternative series gave results in agreement with those of the earlier series increased our confidence in the accuracy of the results reported here.

References

[1] Killingbeck J P and Jones M N 1986 *J. Phys. A: Math. Gen.* **19** 705
[2] Witwit M R M 1991 *J. Phys. A: Math. Gen.* **24** 4535