Hankel-Hadamard analysis of quantum potential $x^2+\lambda x^2/(1+gx^2)$



1985 J. Phys. A: Math. Gen. 18 3593

(http://iopscience.iop.org/0305-4470/18/18/021)

J. Phys. A: Math. Gen. **18** (1985) 3593-3596. Printed in Great Britain

COMMENT

# Hankel–Hadamard analysis of quantum potential $x^2+\lambda x^2/(1+gx^2)$

Carlos R Handy

Department of Physics, Atlanta University, Atlanta, GA 30314, USA

Received 17 April 1985, in final form 4 June 1985

**Abstract.** The Hankel-Hadamard moment determinant analysis of Handy and Bessis is applied to the potential $x^2+\lambda x^2/(1+gx^2)$. Rapidly convergent lower and upper bounds to the ground-state energy and first excited state are obtained. Application of a novel type of Padé analysis allows the determination of all other excited states through an orthogonality quantisation prescription.

In a recent work Handy and Bessis (1985) used the Stieltjes moment theory of Hankel-Hadamard determinants to generate rapidly convergent lower and upper bounds for the ground-state energy of bosonic systems. In a subsequent work Handy and Msezane (1985) extended this technique to first excited states. In addition, through a novel application of Padé analysis the other excited states were also obtained through an orthogonality quantisation condition. The recent interest in the quantum potential $x^2+\lambda x^2/(1+gx^2)$ (Lai and Lin 1982) has prompted us to study this system. Indeed, this problem becomes very simple through our approach. We are able to disprove some of the results of Lai and Lin (1982) as well as those of Bessis and Bessis (1980); however, for the most part our results are consistent with theirs.

Consider the quantum system $-\Psi''+[x^2+\lambda x^2/(1+gx^2)]\Psi = E\Psi$. If one transforms into the function space $\Phi = \exp(-\frac{1}{2}x^2)\Psi$ then a simple recursion relation for the $\Phi$ space Hamburger moments ensues ($\tilde{\mu}(p) = \int \mathrm{d}x\, x^p \Phi$)

$$\tilde{\mu}(p+2) = \frac{\tilde{\mu}(p)[(1+E)+g(p+2)(p+1)-2(p+1)]+p(p-1)\tilde{\mu}(p-2)}{2g(p+3)+\lambda-g(1+E)}. \tag{1}$$

Equation (1) involves only *one* undetermined parameter, $E$, after normalising by $\tilde{\mu}(0)=1$. This was not the case for the $\Psi$ space moments; thus motivating the above transformation. Because a non-negative ground state is known to exist, and it must have finite positive moments, an examination of the zeros of $\tilde{\mu}(2)$'s denominator easily leads to the expression $E_0 = 1-2g$ if $\lambda = -4g-2g^2$. This result for the ground-state energy is derived by Lai and Lin (1982) through slightly more complicated analysis. A similar argument holds for the first excited state. It is simple to argue that from parity the first excited state must be of the form $\Psi_1 = xN_1$, where $N_1$ is a non-negative configuration. Working with the moments of $x^2\exp(-\frac{1}{2}x^2)N_1(x)$ one can obtain $E_1 = 3(1-2g)$ if $\lambda = -4g-6g^2$.

The more effective representation in which to implement a Hankel-Hadamard determinant analysis is in the function space $F(x) = \exp(-\frac{1}{2}x^2)\Psi(x)/(1+gx^2)$. We may denote the ground and first excited states by $\Psi_i(x) = x^i N_i(x)$, for $i = 0, 1$, respectively.

0305-4470/85/183593+04$02.25  

The $N_i(x)$ are non-negative. The recursion relation for the moments of $x^{2i}\exp(-\frac{1}{2}x^2)N_i(x)/(1+gx^2)$ is

$$\tilde{\mu}_{fi}(p+2)=\frac{\tilde{\mu}_{fi}(p)[E-1-2(i+p)+gp(p-1+2i)]+p(p-1+2i)\tilde{\mu}_{fi}(p-2)}{\lambda+g(1+2i-E)+2gp}. \tag{2}$$

An examination of the bounds $0<\tilde{\mu}_{fi}(2)<\infty$, similar to that done for $\tilde{\mu}_i(2)$, leads to the bounds $1+2i<E_i<1+2i+\lambda/g$.

The Stieltjes moment theory of Hankel-Hadamard determinant analysis says that the necessary and sufficient condition for a given set of moments to correspond to a non-negative function measure is that the following inequalities hold:

$$\Delta(0,n)\equiv\begin{vmatrix}\hat{\mu}(0) & \hat{\mu}(1) & \dots & \hat{\mu}(n)\\ \hat{\mu}(n) & \hat{\mu}(n+1) & \dots & \hat{\mu}(2n)\end{vmatrix}>0$$

$$\Delta(1,n)\equiv\begin{vmatrix}\hat{\mu}(1) & \hat{\mu}(2) & \dots & \hat{\mu}(n+1)\\ \hat{\mu}(n+1) & \hat{\mu}(n+2) & \dots & \hat{\mu}(2n+1)\end{vmatrix}>0 \tag{3}$$

where $\hat{\mu}(q)=\tilde{\mu}_{fi}(2q)$, and $0\leqslant n<\infty$.

The Hankel-Hadamard determinants are implicitly $E$ dependent polynomials. The above inequalities define constraints on $E_i$ which are evaluated numerically. These results are given in the tables. Note, for given $N$, all the determinants of order $0\leqslant n\leqslant N$ are considered. Of particular note are the results in table 1. The bounds obtained for $E_{0,1}$ do not concur with the results of Lai and Lin (1982) and Bessis and Bessis (1980).

Once the ground-state and first excited-state values are obtained it is possible to use an orthogonality quantisation condition to obtain the higher excited states (Handy and Msezane 1985). Specifically, one looks at the expressions $G_i(E;E_i)=\int dx\,\Psi_E(x)\Psi_i(x)=\Sigma_{w=0}^{\infty}r^wS_i(w;E;E_i)$, where $r$ is implicitly set at unity. The coefficients are $S_i(w;E;E_i)=\tilde{D}_i(w;E)\,\tilde{\mu}_i(2w;E_i)$. The $\tilde{D}$'s correspond to the $x$-power

**Table 1.** Ground and first excited energy bounds from Hankel-Hadamard analysis. $\lambda=0.1$, $g=2$.

| $N$ | $E_{0N}^{(-)}$ | $E_{0N}^{(+)}$ | $E_{1N}^{(-)}$ | $E_{1N}^{(+)}$ |
|---|---|---|---|---|
| 1 | 1.012 | 1.026 | 3.000 1 | 3.050 1 |
| 2 | 1.015 3 | 1.020 0 | 3.029 1 | 3.035 1 |
| 3 | 1.016 3 | 1.018 4 | 3.031 5 | 3.033 7 |
| 4 | 1.016 7 | 1.017 8 | 3.032 10 | 3.033 20 |
| 5 | 1.016 9 | 1.017 5 | 3.032 45 | 3.033 00 |
| 6 | 1.017 0 | 1.017 4 | 3.032 59 | 3.032 90 |
| 7 | 1.017 1 | 1.017 3 | 3.032 66 | 3.032 85 |
| 8 | 1.017 13 | 1.017 25 | 3.032 70 | 3.032 82 |
| 9 | 1.017 15 | 1.017 22 | 3.032 72 | 3.032 80 |
| 10 | 1.017 16 | 1.017 21 | 3.032 74 | 3.032 79 |
| 11 | 1.017 167 | 1.017 196 | 3.032 75 | 3.032 78 |
| 12 | 1.017 171 | 1.017 191 | 3.032 755 | 3.032 775 |
| 13 | 1.017 174 | 1.017 188 | 3.032 758 | 3.032 772† |
| 14 | 1.017 176 | 1.017 185† | | |

† Estimated values by Lai and Lin $E_0=1.017\,281\,60$, $E_1=3.032\,957\,27$. Estimated values by Bessis and Bessis (1980) $E_0=1.017\,894\,66$, $E_1=3.031\,773$.

**Table 2.** Ground and first excited energy bounds from Hankel-Hadamard analysis $\lambda = 0.1$, $g = 0.1$.

| $N$ | $E_{0N}^{(-)}$ | $E_{0N}^{(+)}$ | $E_{1N}^{(-)}$ | $E_{1N}^{(+)}$ |
|---|---|---|---|---|
| 1 | 1.041 | 1.051 | 3.1 | 3.2 |
| 2 | 1.043 1 | 1.043 3 | 3.12 | 3.13 |
| 3 | 1.043 17 | 1.043 18 | 3.120 | 3.121 |
| 4 | 1.043 173 | 1.043 174 | 3.120 | 3.120 1 |
| 5 | 1.043 173 7 | 1.041 173 8 | 3.120 08 | 3.120 09 |
| 6 | 1.043 173 71 | 1.043 173 72 | 3.120 081 | 3.120 082 |
| 7 | | | 3.120 081 8 | 3.120 081 9 |
| 8 | | | 3.120 081 86 | 3.120 081 87 |
| 9 | | | 3.120 081 864 | 3.120 081 865 |
| | | ($\lambda = 100$, $g = 0.1$) | | |
| 7 | 9.976 15 | 9.976 25 | 29.780 | 29.782 |
| 8 | 9.976 17 | 9.976 19 | 29.781 1 | 29.781 4 |
| 9 | 9.976 179 | 9.976 182 | 29.781 18 | 29.781 22 |
| 10 | 9.976 180 0 | 9.976 180 3 | 29.781 189 | 29.781 195 |
| 11 | 9.976 180 07 | 9.976 180 12 | 29.781 190 8 | 29.781 191 7 |
| 12 | | | 29.781 191 07 | 29.781 191 20 |
| 13 | | | 29.781 191 10 | 29.781 191 13 |

**Table 3.** Ground and first excited energy bounds from Hankel-Hadamard analysis $\lambda = 100$, $g = 2$.

| $N$ | $E_{0N}^{(-)}$ | $E_{0N}^{(+)}$ | $E_{1N}^{(-)}$ | $E_{1N}^{(+)}$ |
|---|---|---|---|---|
| 3 | 8 (5)† | 10 (19)† | 20 | 28 |
| 4 | 8.4 (6) | 9.3 (14) | 21 | 26 |
| 5 | 8.6 (7) | 9.0 (12) | 22.7 | 24.8 |
| 6 | 8.67 (7.5) | 8.88 (10.5) | 23.1 | 24.3 |
| 7 | 8.71 (8.2) | 8.83 (9.6) | 23.3 | 24.1 |
| 8 | 8.73 (8.35) | 8.80 (9.3) | 23.51 | 23.95 |
| 9 | 8.74 (8.5) | 8.78 (9.1) | 23.60 | 23.87 |
| 10 | 8.747 (8.5) | 8.772 (9.0) | 23.65 | 23.84 |
| 11 | 8.751 (8.6) | 8.767 (8.95) | 23.68 | 23.80 |
| 12 | 8.754 (8.67) | 8.764 (8.87) | 23.70 | 23.78 |
| 13 | 8.755 | 8.762 | 23.71 | 23.77 |
| 14 | 8.756 | 8.761 | 23.72 | 23.76 |
| 15 | 8.756 | 8.760 | 23.73 | 23.75 |
| 16 | 8.7572 | 8.7594 | | |

† Results from Hankel-Hadamard analysis for representation in equation (1).

series expansion of $\exp(\frac{1}{2}x^2)(\Psi(x)/x^t)$, and easily obtainable. One then Padé analyses (Baker 1975) $\Sigma_0^W r^w S(w) = P'_B(E; r=1)/P''_B(E; r=1)$, where the Padé polynomials have $r$ degree '$B$' ($W = 2B$). The zeros of the Padé provide good estimates for the excited-state spectrum. Note, spurious zeros appear and are ignored. The non-spurious zeros define consistent eigen energies. All numerical analysis was done on the CRAY using single precision arithmetic.

**Table 4.** Lower excited even parity states from Padé of $G_0(E; E_0)$.

| $W$ | $E_0 = 1.017\,180$ ($\lambda = 0.1, g = 2$) | $E_0 = 1.043\,173\,71$ ($\lambda = 0.1, g = 0.1$) | $E_0 = 9.976\,180\,095$ ($\lambda = 100, g = 0.1$) | $E_0 = 8.758\,278\,63$ ($\lambda = 100, g = 2$) |
|---|---|---|---|---|
| 4 | 5.0473 | 5.1816<br>9.1928 | 49.3249 | 35.0187 |
| 6 | 5.0397 | 5.1803<br>9.2698 | 49.2525 | 34.2717 |
| 8 | 5.0369<br>8.5592 | 5.1815<br>9.2728 | 49.2929 | 34.0878 |
| 10 | 5.0357<br>8.8658 | 5.1810<br>9.2761 | 49.2917 | 34.0453 |
| 12 | 5.0351<br>8.9594 | 5.1818<br>9.2719 | 49.2877 | 34.0402 |
| 14 | 5.0347<br>8.9977 | 5.1812<br>9.2729 | 49.2962 | 34.0396 |
| 16 | 5.0344<br>9.0157 | 5.1809<br>9.2750 | 49.2930 | 34.0272 |
| 18 | 5.0341<br>9.0250 | 5.1815<br>9.2718 | 49.2940 | 34.0023 |
| 20 | 5.0339<br>9.0302 | 5.1812<br>9.2726 | 49.2922 | 33.8940 |

**Table 5.** Lower excited odd parity states ($E > E_1$) from Padé of $G_1(E; E_1)$.

| $W$ | $E_1 = 3.032\,765$ ($\lambda = 0.1, g = 2$) | $E_1 = 3.120\,081\,865$ ($\lambda = 0.1, g = 0.1$) | $E_1 = 29.781\,191\,115$ ($\lambda = 100, g = 0.1$) | $E_1 = 23.743\,326\,04$ ($\lambda = 100, g = 2$) |
|---|---|---|---|---|
| 4 | 7.0692 | 7.2324 | 70.2346 | 40.4851 |
| 6 | 7.0500 | 7.2309 | 68.6057 | 39.9923 |
| 8 | 7.0434 | 7.2321 | 68.5160 | 39.9679 |
| 10 | 7.0406 | 7.2312 | 68.5133 | 39.9295 |
| 12 | 7.0392 | 7.2306 | 68.5123 | 39.6311 |
| 14 | 7.0385 | 7.2314 | 68.5143 | 38.7539 |
| 16 | 7.0380 | 7.2311 | 68.5131 | 38.2201 |
| 18 | 7.0377 | 7.2307 | 68.5106 | 38.0666 |
| 20 | 7.0375 | 7.2314 | 68.5140 | 38.9605 |

The author expresses his appreciation to Professor Frank Cummings for bringing this problem to his attention. Support from grants NSF RII-8312 and DOE DE-AC05-840R21400 is acknowledged.

## References

Baker G A Jr 1975 *Essentials of Pade Approximants* (New York: Academic)
Bessis N and Bessis G 1980 *J. Math. Phys.* **21** 2780
Handy C R and Bessis D 1985 *Phys. Rev. Lett.* **55** 931
Handy C R and Msezane A Z 1985 unpublished, Atlanta University
Lai C S and Lin H E 1982 *J. Phys. A: Math. Gen.* **15** 1495