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A moment equation reformulation of Rayleigh–Ritz theory

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Abstract. We present a moment equation Rayleigh–Ritz (RR) variational theory for the ground-state energy. An extended Fourier transform space can be defined through the moment equation corresponding to a given Schrödinger Hamiltonian. Within this extended space, we can implement a variational ansatz with respects to configurations of the form $\tilde{\Psi}_{E,\mu}(k) = \sum_l \tilde{\mathcal{T}}_l(E,k)\mu_l$ in which the energy-dependent functions $\tilde{\mathcal{T}}_l(E,k)$: (i) satisfy the momentum space Schrödinger equation; (ii) are uniquely prescribed; (iii) are (most likely) non-integrable; and (iv) yield the L^2 physical solution for physical E and μ_l values. On the basis of this representation, one can minimize the energy expectation value $\mathcal{E}(E,\ldots,\mu_l,\ldots)$ with respects to the E and missing moment variables, μ_l. The proposed approach is in sharp contrast to traditional configuration-space RR implementations in which the selection of a variational basis is not manifest *a priori*, particularly for problems of spatial dimension greater than one. The analysis of one- and two-dimension problems is presented.

1. Introduction

Many Schrödinger Hamiltonians (including all rational fraction potential problems) can be transformed into a linear moment equation representation:

$$\sum_{i=s}^{d} C(E,p,i)\mu(p+i) = 0 \qquad 0 \leqslant p < \infty \tag{1.1}$$

involving the moments of the wavefunction $\mu(p) \equiv \int x^p \Psi(x)\,\mathrm{d}x$, and the energy, E.

Since the late 1970s various researchers have developed different quantization approaches for solving moment equation representations of the Schrödinger equation. Besides the academic interest in such matters, a more practical incentive has been the recognition that momentum space based quantization offers a more appropriate setting in which to solve strongly coupled/singular perturbation type problems and the attendant interplay of multiscale interactions. An important example is the use of moment quantization methods (Handy *et al* 1988) to solve the famous quadratic Zeeman effect for superstrong magnetic fields, amply reviewed and analyzed in the work of Le Guillou and Zinn-Justin (1983) (hereafter referred to as LZ). The former approach was able to easily confirm the more intricate conformal analysis of LZ.

Quantization is a global problem. Non-local representations involving spatially extensive 'dynamical' variables, such as moments, should be more sensitive to multiscale features of a system, from large spatial scale contributions to smaller ones. Handy and Murenzi (1995) have shown that a moment equation representation quantization faciliates the multiscale recovery of wavefunctions, from first principles, through continuous wavelet transform

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methods (Chui 1992). Wavelet transform analysis has been very useful in signal and image processing because of its ability to effectively achieve simultaneous position and frequency localization; thereby expediting the multiscale recovery of abruptly varying signals and images. The direct extension of continuous wavelet transform methods to quantum mechanics has been difficult because arbitrary potential functions (including those of rational fraction form) do not permit a simple transformation of the Schrödinger equation into a wavelet equation. Nevertheless, through a moment-equation representation one can circumvent these difficulties and recover the bound-state wavefunction, systematically, from large spatial scales down to smaller scales. No other quantum mechanics formalism offers this flexibility.

Moment quantization methods of comparative relevance to the present work include those of Blankenbeckler, DeGrand, and Sugar (1980). Their quantization of (1.1) is achieved by using certain asymptotic relations to constrain the moments and energy. Additional works by Killingbeck *et al* (1985), Fernandez (1992), Fernandez and Ogilvie (1993) and Witwit (1995) (and references cited therein) develop perturbation theory methods within the moment equation representation. One immediate advantage of their collective approach is that explicit reference to the wavefunction's perturbative structure is not required. That is, one can easily generate the perturbative expansion for the energy directly.

In contrast to the preceding eigenenergy estimation methods the works by Handy and Bessis (1985) and Handy *et al* (1988) exploit theorems from the classic moment problem (Shohat and Tamarkin 1963) in order to generate rapidly converging lower and upper bounds to the ground-state energy. This bounding theory is referred to as the eigenenergy moment method (EMM).

In this work, we develop a new moment equation quantization method not contained in any of the aforementioned approaches. It corresponds to a special kind of momentum space Rayleigh–Ritz variational analysis in which the effective 'basis' functions are predetermined through (1.1). This analysis holds for multidimensional problems as well. An example is discussed in this work.

Re-examining equation (1.1), we note that the energy dependent coefficients, as well as the $\{s, d\}$ indices are problem dependent. The algebraic degree of the configuration space potential function, d (usually, $d > 2$), determines the differential order of the associated momentum space differential equation for the Fourier transformed wavefunction

$$\tilde{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int \mathrm{e}^{-\mathrm{i}kx} \Psi(x)\, \mathrm{d}x = \frac{1}{\sqrt{2\pi}} \sum_{p=0}^{\infty} (-\mathrm{i}k)^p \frac{\mu(p)}{p!}.$$

Viewed as an initial value problem, one can encounter more initialization variables $(\mathrm{d}^j \tilde{\Psi}(k)/\mathrm{d}k^j|_{k=0} = (1/\sqrt{2\pi})(-\mathrm{i})^j \mu(j), 0 \leqslant j \leqslant d)$ than the usual two associated with second-order, one-dimensional, problems ($\Psi(0)$ and $\mathrm{d}\Psi(x)/\mathrm{d}x|_{x=0}$). The large number of such variables is the basic obstacle encountered in any moment equation based quantization scheme. From the above, it is clear that the momentum space initialization variables are essentially the first d moments. These are refered to, hereafter, as *missing moments*.

In this work, we examine the effectiveness of a Rayleigh–Ritz variational ansatz in which the missing moments become the variational parameters, together with the variable energy parameter, E. This approach is quite unique because it requires that one work in an extended function space with no obvious x-configuration space counterpart. Thus, for the problems considered here, our momentum space variational analysis will be done with respects to configurations of the form

$$\tilde{\Psi}_{E,\mu}(k) = \sum_{l=0}^{d-1} \mu(l) \tilde{\mathcal{I}}_l(E, k) \tag{1.2}$$

where the energy parameter dependent functions $\tilde{\mathcal{T}}_l(E,k)$ are analytic and known (in terms of their power series expansion). More importantly, each of these functions is a solution to the momentum space Schrödinger equation, $\tilde{\mathcal{H}}\tilde{\Psi}(k) = E\tilde{\Psi}(k)$. Generally, the analyticity property holds for systems where the x-configuration space bound state falls off faster than a simple exponential ($\exp(-\kappa x), 0 < \kappa < \infty$). The same also applies for unphysical E values, as can be verified through a simple application of the ratio test (refer to section 2). In this preliminary work, we do not discuss singular potential problems nor those violating the indicated conditions.

It is important to appreciate that for physical (bound state) values for the energy and missing moment variables, E_{b} and $\mu_{\mathrm{b}}(l)$, respectively, the *exact* bound state is given by $\tilde{\Psi}_{E_{\mathrm{b}},\mu_{\mathrm{b}}}(k) = \sum_{l=0}^{d-1}\mu_{\mathrm{b}}(l)\tilde{\mathcal{T}}_l(E_{\mathrm{b}},k)$, and must vanish asymptotically, $\mathrm{Lim}_{k\to\infty}\tilde{\Psi}_{\mathrm{b}}(k) \to 0$. Even then, each $\tilde{\mathcal{T}}_l(E_{\mathrm{b}},k)$ can be asymptotically unbounded, $\mathrm{Lim}_{k\to\infty}\tilde{\mathcal{T}}_l(E_{\mathrm{b}},k) \to \infty$ (note the trivial observation that a bounded function, such as e^{-k^2}, can be written as the sum of two, or more, unbounded functions: $\mathrm{e}^{-k^2} = [\mathrm{e}^{k^2} + \mathrm{e}^{-k^2}] - \mathrm{e}^{k^2}$).

For unphysical energy and/or missing moment values, the $\tilde{\Psi}_{E,\mu}(k)$ configuration should be unbounded as well. In general, these unphysical solutions have no immediate x-configuration space counterpart. Indeed, unphysical solutions to the x-configuration space Schrödinger equation are unbounded, with infinite power moments, and generally do not admit a Fourier transform. Therefore, the $\tilde{\mathcal{T}}_l(E,k)$ momentum space expressions do not appear to be any kind of generalized Fourier transforms for such unphysical x-configuration space solutions.

The principal challenge in implementing our moment equation representation Rayleigh–Ritz variational analysis will be in defining the momentum space energy expectation value

$$\mathcal{E}[E,\boldsymbol{\mu}] \equiv \frac{\langle\tilde{\Psi}_{E,\mu}|\tilde{\mathcal{H}}|\tilde{\Psi}_{E,\mu}\rangle}{\langle\tilde{\Psi}_{E,\mu}|\tilde{\Psi}_{E,\mu}\rangle} \tag{1.3}$$

while utilizing the power series expansions for the $\tilde{\mathcal{T}}_l(E,k)$ functions. This is discussed in the following sections. In so far as the small k power series expansion reflects the large scale (global) x-configuration bound state, and quantization is basically a global problem, a reasonable regulation prescription for evaluating $\mathcal{E}[E,\boldsymbol{\mu}]$ should still yield satisfactory ground-state energy estimates. This is the case for all the problems investigated here.

One of the unique features of our variational approach is that the energy expectation value, $\mathcal{E}$, depends on the energy variable, E. Let E^*, μ^* denote the parameter values corresponding to the global minimum for the (regulated) $\mathcal{E}[E,\boldsymbol{\mu}]$ function:

$$\mathrm{Min}_{E,\mu}\,\mathcal{E}[E,\boldsymbol{\mu}] \equiv \mathcal{E}[E^*,\boldsymbol{\mu}^*] \equiv \mathcal{E}^*. \tag{1.4}$$

One expects that a satisfactory regulating prescription for $\mathcal{E}[E,\boldsymbol{\mu}]$ is one that yields $E^* \approx \mathcal{E}^*$. Again, this is verified by our analysis.

Traditional implementations of Rayleigh–Ritz variational analysis work with an approximate basis set $\sum_i c_i\mathcal{B}_i(x)$ in which the basis functions are chosen as simply as possible and made to satisfy important features of the desired ground-state wavefunction. Furthermore, these basis functions are usually L^2 integrable. In our analysis, we work with 'basis' functions that are predetermined by the system equation (equation (1.1)) and (most likely) unbounded solutions (in power series form) to the momentum space Schrödinger equation.

Clearly, one could implement a Rayleigh–Ritz variational analysis in x-configuration space utilizing, when admissible, a Taylor series expansion for the wavefunction. However, this cannot yield any reasonable values for the ground-state energy because this process is highly local and does not capture any of the global structure essential to addressing eigenenergy quantization. A simple example of this is provided towards the end of section 3.

2. Moment equation variational formalism

For simplicity, consider the rescaled $2Q$ anharmonic oscillator problem

$$-\epsilon^2\frac{d^2\Psi}{dx^2}+[mx^2+gx^{2Q}]\Psi(x)=E\Psi(x) \tag{2.1}$$

with

$$\tilde{\mathcal{H}}=\epsilon^2k^2-m\frac{d^2}{dk^2}+g(-1)^Q\frac{d^{2Q}}{dk^{2Q}}$$

as the corresponding Fourier space Hamiltonian. The ϵ^2 parameter is included for reasons clarified below, although it is set to unity ($\epsilon\equiv 1$). Restricting ourselves to the symmetric configurations, define the even order Hamburger power moments by $u(p)=\int_{-\infty}^{\infty}dx\,x^{2p}\Psi(x)$. Upon integrating both sides of (2.1) by $\int dx\,x^{2p}$, and performing the necessary integration by parts, we obtain the moment equation

$$u(p+Q)=g^{-1}\big(2p(2p-1)\epsilon^2\,u(p-1)+Eu(p)-mu(p+1)\big) \tag{2.2}$$

for $p\geqslant 0$. This corresponds to a linear, homogeneous, finite-difference equation of order Q, since the initialization moments $\{u(0),u(1),\ldots,u(Q-1)\}$ must be specified before the remaining moments can be generated. They will be referred to as *missing* moments. The energy appears as an arbitrary parameter, E. The linear dependence on the missing moments is expressed through the relation

$$u(p)=\sum_{l=0}^{Q-1}M_E(p,l)u(l) \tag{2.3}$$

where $M_E(i,j)=\delta_{i,j}$, for $0\leqslant i,j\leqslant Q-1$. The $M_E(p,l)$ coefficients, for fixed l, are recursively generated through an equation identical to (2.2).

Through a simple asymptotic analysis, the leading behaviour for an arbitrary u-solution is of the form

$$\frac{u(p+1)}{u(p)}\approx\left[\frac{\epsilon^2}{g}(2p)^2\right]^{1/(Q+1)}.$$

This ensures that the (Fourier transform) power series

$$\tilde{\Psi}(k)=\frac{1}{\sqrt{(2\pi)}}\sum_{p=0}\frac{u(p)}{(2p)!}(-ik)^{2p}$$

has an infinite radius of convergence, as verified through the ratio test, and is therefore entire. The same holds for

$$\tilde{\mathcal{T}}_l(E,k)=\frac{1}{\sqrt{(2\pi)}}\sum_{p=0}\frac{\mathcal{M}_E(p,l)}{(2p)!}(-ik)^{2p}.$$

In particular

$$\tilde{\Psi}(E,\boldsymbol{u};k)=\sum_{l=0}^{Q-1}u(l)\tilde{\mathcal{T}}_l(E,k). \tag{2.4}$$

The two expressions $\tilde{\Psi}(k)$ and $\tilde{\Psi}(E, \boldsymbol{u}; k)$ are identical; however, the latter emphasizes the implicit E and $\boldsymbol{u} \equiv (u(0), \ldots, u(Q-1))$ dependence.

For physical (bound state) energy and missing moments values, hereafter referred to as E_{b} and $\boldsymbol{u}_{\mathrm{b}}$, $\tilde{\Psi}(E_{\mathrm{b}}, \boldsymbol{u}_{\mathrm{b}}; k)$ is integrable with a finite Hamiltonian expectation value

$$\mathcal{E}[E_{\mathrm{b}}, \boldsymbol{u}_{\mathrm{b}}] \equiv \frac{\langle \tilde{\Psi}(E_{\mathrm{b}}, \boldsymbol{u}_{\mathrm{b}}) | \tilde{\mathcal{H}} | \tilde{\Psi}(E_{\mathrm{b}}, \boldsymbol{u}_{\mathrm{b}}) \rangle}{\langle \tilde{\Psi}(E_{\mathrm{b}}, \boldsymbol{u}_{\mathrm{b}}) | \tilde{\Psi}(E_{\mathrm{b}}, \boldsymbol{u}_{\mathrm{b}}) \rangle} .$$

Unphysical Ψ configurations do not satisfy the moment equation, since their power moments are infinite. Nevertheless, the moment equation contains more moment-solutions, for arbitrary E and $\{u(0), \ldots, u(Q-1)\}$, than are physically allowed.

In general, for arbitrary energy and missing moment values, $\tilde{\Psi}(E, \boldsymbol{u}, k)$ may not be integrable, and thus $\mathcal{E}[E, \boldsymbol{u}]$ need not exist. However, with respects to our moments' Rayleigh–Ritz implementation, this does not matter, as will be clarified below.

From the perspective of distribution theory, it is possible that the inverse Fourier transform of $\tilde{\Psi}(E, \boldsymbol{u}, k)$ could involve 'integrable' generalized functions. In particular, for the case $\epsilon \to 0$, the general moment solution corresponds to $u(p) = \sum_{j=0}^{2Q-1} A_j \tau_j^{2p}$, where τ_j is a turning point solution $m\tau_j^2 + g\tau_j^{2Q} = E$. Thus the inverse Fourier transform becomes a sum of Dirac measures:

$$\frac{1}{\sqrt{(2\pi)}} \int_{-\infty}^{\infty} \mathrm{d}k \ \exp(\mathrm{i}kx) \tilde{\Psi}(E, k) = \sum_{j=0}^{2Q-1} A_j \delta(x - \tau_j) .$$

For the physical energy and missing moment values, we cannot compute $\mathcal{E}[E_{\mathrm{b}}, \boldsymbol{u}_{\mathrm{b}}]$ by truncating the $\tilde{\Psi}(E_{\mathrm{b}}, \boldsymbol{u}_{\mathrm{b}}; k)$ power series at some finite order in k and imposing a momentum space cut-off regulator (i.e. $\int_{-\Lambda}^{\Lambda} \mathrm{d}k$). This is because there would be no guarantee of consistently generating upper bounds through a Rayleigh–Ritz variational analysis. Instead, we must define an intermediate transformation : $\tilde{\Psi}(k) = \left[\sum_{j=0}^{\infty} C_j (-\mathrm{i}k)^{2j}\right](1/s)\tilde{G}(k/s)$, where $\tilde{G}(k/s)$ falls off exponentially at infinity, $\tilde{G}(k)^{-1}$ is an arbitrary entire function, and s is an arbitrary scaling parameter.

The C-expansion defines the entire function $\tilde{C}_{E_{\mathrm{b}}}(k)$. One can now replace the $\tilde{\Psi}(E_{\mathrm{b}}, \boldsymbol{u}_{\mathrm{b}})$ expression in the energy expectation value with the truncated C-expansion: $\tilde{\Psi}(E_{\mathrm{b}}, \boldsymbol{u}_{\mathrm{b}}; k) \approx \left[\sum_{j=0}^{\mathcal{P}} C_j (-\mathrm{i}k)^{2j}\right](1/s)\tilde{G}(k/s)$. If $\tilde{G}(k)$ asymptotically approaches zero fast enough (so that the integration and series summation appearing in $\mathcal{E}$ can be interchanged) then one will obtain convergence to the true ground-state energy in the limit $\mathcal{P} \to \infty$. If this is not the case, then a reasonable choice of $\tilde{G}(k)$ should still yield good estimates for the ground-state energy as the $\mathcal{P}$-expansion order is increased.

The C-coefficients satisfy the relation

$$\sum_{j=0}^{p} C_j s^{-[1+2(p-j)]} \gamma_{p-j} = \frac{u_{\mathrm{b}}(p)}{(2p)!} \tag{2.5}$$

where

$$\tilde{G}(k) = \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} \gamma_n (-\mathrm{i}k)^{2n} .$$

Clearly, C_p is recursively generated from the lower order coefficients, and they are linearly dependent on the u-moments. In particular, we may replace $u(p) \to M_E(p, l)$ and thereby define the corresponding Cs as $C_{E;j}^{(l)}$. The associated function is referred to as $\tilde{C}_E^{(l)}(k) \equiv \sum_{j=0}^{\infty} C_{E;j}^{(l)}(-\mathrm{i}k)^{2j}$. We reemphasize that even though the $\tilde{C}_{E_\mathrm{b}}^{(l)}(k)$'s may not be integrable individually, collectively they define an integrable function, $\tilde{C}_{E_\mathrm{b}}(k) = \sum_l u_\mathrm{b}(l)\tilde{C}_{E_\mathrm{b}}^{(l)}(k)$, for physical E_b and $\boldsymbol{u}_\mathrm{b}$. The power series expansion of $\tilde{C}_{E_\mathrm{b}}(k)$ is the sum of the power series for each $\tilde{C}_{E_\mathrm{b}}^{(l)}(k)$.

Let us now define

$$\tilde{\Psi}_{\mathcal{P}}(E, \boldsymbol{u}; k) \equiv \left[\sum_{l=0}^{Q-1} u(l)\left(\sum_{j=0}^{\mathcal{P}} C_{E;j}^{(l)}(-k^2)^j\right)\right]\frac{1}{s}\tilde{G}(k/s)\,. \tag{2.6}$$

The $\mathcal{E}$-expectation value for such $\tilde{\Psi}_{\mathcal{P}}(E, \boldsymbol{u}; k)$ configurations exist. We may therefore minimize over the E and $\boldsymbol{u}$ variables. We have

$$\mathcal{E}_{\mathcal{P}}[E, \boldsymbol{u}] \equiv \mathcal{E}[\tilde{\Psi}_{\mathcal{P}}(E, \boldsymbol{u})]$$

or

$$\mathcal{E}_{\mathcal{P}}[E, \boldsymbol{u}] = \frac{\sum_{l_1,l_2=0}^{Q-1} u(l_1)\mathcal{G}_E(l_1, l_2)u(l_2)}{\sum_{l_1,l_2=0}^{Q-1} u(l_1)\mathcal{D}_E(l_1, l_2)u(l_2)} \tag{2.7}$$

where

$$\mathcal{G}_E(l_1, l_2) = s^{-2}\sum_{j_1,j_2=0}^{\mathcal{P}} C_{E;j_1}^{(l_1)}\left\langle(-k^2)^{j_1}\tilde{G}(k/s)\middle|\tilde{\mathcal{H}}\middle|(-k^2)^{j_2}\tilde{G}(k/s)\right\rangle C_{E;j_2}^{(l_2)}$$

and

$$\mathcal{D}_E(l_1, l_2) = s^{-2}\sum_{j_1,j_2=0}^{\mathcal{P}} C_{E;j_1}^{(l_1)}\left\langle(-k^2)^{j_1}\tilde{G}(k/s)\middle|(-k^2)^{j_2}\tilde{G}(k/s)\right\rangle C_{E;j_2}^{(l_2)}.$$

Note that for one-dimensional problems, the dimension of the $\mathcal{G}_E(l_1, l_2)$ matrix is fixed at Q.

The denominator quadratic form in (2.7) defines a positive matrix. As such, we may determine its associated positive square root matrix $\mathcal{D}_E = \mathcal{S}_E^2$ and redefine $\boldsymbol{v} \equiv \mathcal{S}_E\boldsymbol{u}$. Consequently, $\mathcal{E}_{\mathcal{P}}[E, \boldsymbol{u}] = \langle\boldsymbol{v}|\mathcal{S}_E^{-1}\mathcal{G}_E\mathcal{S}_E^{-1}|\boldsymbol{v}\rangle/\langle\boldsymbol{v}|\boldsymbol{v}\rangle$. The minimum over the $\boldsymbol{v}$ vector space corresponds to the smallest eigenvalue for the $\mathcal{S}_E^{-1}\mathcal{G}_E\mathcal{S}_E^{-1}$ matrix. Thus we have

$$\mathrm{Min}_{\boldsymbol{u}}\,\mathcal{E}_{\mathcal{P}}[E, \boldsymbol{u}] = \Lambda_{\mathcal{P}}(E) \equiv \text{smallest eigenvalue of }\left(\mathcal{S}_E^{-1}\mathcal{G}_E\mathcal{S}_E^{-1}\right). \tag{2.8}$$

The full implementation of the moment equation based Rayleigh Ritz variation also requires varying E; therefore we have

$$E_{\mathrm{ground}} \leqslant \mathrm{Min}_E\,\Lambda_{\mathcal{P}}(E). \tag{2.9}$$

As previously suggested, any valid interpretation of the above Fourier space formalism in configuration space will require significant use of distribution theory. Despite this, we can symbolically perform the same manipulations in configuration space, facilitating the derivation of useful formulae. Thus, we may work with the symbolic inverse Fourier transform of $\tilde{\Psi}(k)$ which we take to be $\Psi(E, \boldsymbol{u}, x) \equiv \sum_{l=0}^{Q-1} u(l)\mathcal{T}_l(E, x)$. The expression

$\mathcal{T}_l(E,x)$ implicitly refers to the limiting form ($\mathcal{P}\to\infty$) of the inverse Fourier transform of the expansion $(\sum_{j=0}^{\mathcal{P}} C_{E;j}^{(l)}(-k^2)^j)s^{-1}\tilde{G}(k/s)$. The moments of $\mathcal{T}_l(E,x)$ correspond to $\int_{-\infty}^{\infty}\mathrm{d}x\, x^{2p}\mathcal{T}_l(E,x) = M_E(p,l)$. We can take $\mathcal{T}_l(E,x) = (\sum_{j=0}^{\infty} C_{E;j}^{(l)}\partial_x^{2j})\, G(sx)$, where G is the inverse Fourier transform of $\tilde{G}$. It then follows that

$$M_E(p,l) = \sum_{j=0}^{p} C_j^{(l)}[E]\frac{(2p)!}{(2(p-j))!}\Gamma_s(p-j)$$

where

$$\Gamma_s(p-j) = \int \mathrm{d}x\, x^{2(p-j)}G(sx) = (2[p-j])!\, s^{-[1+2(p-j)]}\gamma_{p-j}\,.$$

3. Numerical examples

We will consider the one-dimensional potentials corresponding to the quartic, sextic, and octic anharmonic oscillators ($Q = 2, 3, 4$, respectively). In addition, the two-dimensional potential $V(x,y) = x^2 + y^2 + \lambda(xy)^2$ will also be considered. In all cases, $G(s\boldsymbol{x}) = \exp(-s^2|\boldsymbol{x}|^2)$. For the one-dimensional cases, expressions of the form

$$\mathcal{I}(l_1,l_2,\sigma,\rho) = \sum_{i_1,i_2=0}^{\mathcal{P}} C_{E;i_1}^{(l_1)}C_{E;i_2}^{(l_2)}\int_{-\infty}^{\infty}\mathrm{d}x\,\left(\partial_x^{2i_1+\sigma}\exp(-(sx)^2)\right)x^\rho\left(\partial_x^{2i_2+\sigma}\exp(-(sx)^2)\right)$$

for $\sigma = 0, 1$ and $\rho \leqslant 2Q$, are required. Substituting

$$\partial_x^{2i_k+\sigma}\exp(-(sx)^2) = \partial_{\delta_k}^{2i_k+\sigma}\exp(-(s[x+\delta_k])^2) \qquad \text{for } k = 1,2$$

and taking $\delta_k \to 0$ after doing the integral gives the relation

$$\begin{aligned}\int_{-\infty}^{\infty}&\mathrm{d}x\,\left(\partial_x^{2i_1+\sigma}\exp(-(sx)^2)\right)x^\rho\left(\partial_x^{2i_2+\sigma}\exp(-(sx)^2)\right)\\ &= s^{2(i_1+i_2+\sigma)-1-\rho}\sum_{n_1=0}^{2i_1+\sigma}\sum_{n_3=0}^{2i_2+\sigma}\frac{(-2)^{n_1+n_3}(-1)^{n_2+n_4}(2i_1+\sigma)!\ (2i_2+\sigma)!}{\sqrt{2}^{1+\rho+n_1+n_3}\prod_{k=1}^{4}n_k!}\\ &\quad\times\Omega\left(\frac{\rho+n_1+n_3}{2}\right)\end{aligned}$$

where $n_1 + 2n_2 = 2i_1 + \sigma$, $n_3 + 2n_4 = 2i_2 + \sigma$ (both n_2 and n_4 must also be positive), and $\Omega(n) = \int \mathrm{d}x\, x^{2n}\exp(-x^2) = ((2n-1)!!/2^n)\sqrt{\pi}$.

In the two-dimensional problem case, the moment equation for $x \leftrightarrow -x$ and $y \leftrightarrow -y$ symmetric configurations, $u(p,q) = \int\int \mathrm{d}x\,\mathrm{d}y\, x^{2p}y^{2q}\Psi(x,y)$, is

$$\begin{aligned}\lambda u(p+1,q+1) &= Eu(p,q) - u(p+1,q) - u(p,q+1) + 2p(2p-1)u(p-1,q)\\ &\quad + 2q(2q-1)u(p,q-1)\end{aligned}\qquad(3.1)$$

where $u(p,q) = u(q,p)$ for the ground state. The missing moments are $\{u(l,0)|0 \leqslant l < \infty\}$. We have that $u(p,q) = \sum_{l=0} M_E(p,q,l)u(l,0)$, where $M_E(i,0,j) = M_E(0,i,j) =$

$\delta_{i,j}$. All of the moments corresponding to $0 \leqslant p, q \leqslant \mathcal{P}$ depend only on the missing moments $u(l, 0)$ for $0 \leqslant l \leqslant \mathcal{P}$.

Using the symbolic representation $\Psi(x, y) = \sum_{l=0} u(l, 0)\mathcal{T}_l[E, x, y]$ where

$$\mathcal{T}_l[E, x, y] = \sum_i \sum_j C^{(l)}_{E;i,j} \partial_x^{2i} \partial_y^{2j} \exp(-(sx)^2 - (sy)^2)$$

we obtain

$$\sum_{i=0}^{p} \sum_{j=0}^{q} C^{(l)}_{E;i,j} \frac{(2p)!(2q)!\Gamma(p-i)\Gamma(q-j)}{[2(p-i)]![2(q-j)]!} = M_E(p, q, l)\,.$$

Hence the $C^{(l)}_{E;i,j}$'s are obtainable recursively as in the one-dimensional case. The relevant integral expressions for calculating the Hamiltoninan expectation value can be computed in a manner similar to that for the one-dimensional problems.

Table 1. Moment equation Rayleigh–Ritz variational analysis.

Potential	E^*	$\mathcal{E}^*$	$\mathcal{P}$	E_{ground}
$x^2 + x^4$	1.392 337 92	1.392 351 74	8	1.392 351 642[a]
$x^2 + x^6$	1.436 12	1.435 654 6	10	1.435 624 619[a]
$x^2 + x^8$	1.490 9	1.491 072	15	1.491 019 895[a]
$x^2 + y^2 + (xy)^2$	2.195 89	2.195 965	9	2.195 918 085[b]

[a]Handy (1996).
[b]Vrscay and Handy (1989).

The results for all four examples are given in table 1. In each case, as the order of the calculation, $\mathcal{P}$, increases, the moment RR estimates monotonically converge to the true value (cited in the last column of table 1). However, such monotonic behaviour need not always be the case. We contrast the variational results (see equation (1.4) for clarification of E^* and $\mathcal{E}^*$) with the more exact answers found in the literature. In all cases $s = 1$ and all other parameters also set to unity ($m = g = \lambda = 1$). The results for the $x^2 + x^6$ potential show that the E^* value does not necessarily define a lower bound to the ground-state energy. In the other three cases, it does give a lower bound.

By way of comparison, we tested the effectiveness of a Rayleigh Ritz ansatz for the anharmonic potentials $(x^2 + gx^{2Q})$ utilizing functions of the form $\Psi(x) \approx \left(\sum_{j=0}^{\mathcal{P}} D_{E;j} x^{2j}\right) \exp(-x^2)$, where the D-expansion represents the power series expansion obtained after replacing the wavefunction with the representation $\Psi(x) = D(x)\exp(-x^2)$. The recursion relation for the $D_{E;j}$ coefficients is given by $D_0 \equiv 1$, $D_1 = \frac{1}{2}(2 - E)$,

$$D_{i+1} = \frac{(8i + 2 - E)D_i - 3D_{i-1}}{2(i+1)(2i+1)} \tag{3.2a}$$

for $1 \leqslant i \leqslant Q - 1$, and

$$D_{i+1} = \frac{(8i + 2 - E)D_i - 3D_{i-1} + D_{i-Q}}{2(i+1)(2i+1)} \tag{3.2b}$$

for $i \geqslant Q$.

The energy expectation value involves the simple expression

$$\mathcal{E}_{2Q}^{(\mathcal{P})}(E) = \frac{\left\langle \sum_{i=0}^{\mathcal{P}} D_i x^{2i} \mathrm{e}^{-x^2} | -\partial^2 + x^2 + x^{2Q} | \sum_{j=0}^{\mathcal{P}} D_j x^{2j} \mathrm{e}^{-x^2} \right\rangle}{\left\langle \sum_{i=0}^{\mathcal{P}} D_i x^{2i} \mathrm{e}^{-x^2} | \sum_{j=0}^{\mathcal{P}} D_j x^{2j} \mathrm{e}^{-x^2} \right\rangle} . \tag{3.3}$$

The numerator and denominator are given by the expressions

$$\sum_{i,j=0}^{\mathcal{P}} D_i D_j \left(4ij\mathcal{I}(i+j-1) + 5\mathcal{I}(i+j+1) - 4(i+j)\mathcal{I}(i+j) + \mathcal{I}(i+j+Q)\right)$$

and $\sum_{i,j=0}^{\mathcal{P}} D_i D_j \mathcal{I}(i+j)$, respectively, where $\mathcal{I}(n) \equiv \int_{-\infty}^{+\infty} x^{2n} \exp(-2x^2)$, $\mathcal{I}(0) = \sqrt{\pi/2}$, and $\mathcal{I}(n) = \frac{1}{4}(2n-1)\mathcal{I}(n-1)$. The entire procedure mimics that developed previously in the Fourier-moment representation.

Unlike the moment formulation in which E and the missing moments are variational parameters, the present configuration space analysis only involves E as a variational parameter. As such, below we cite the $\mathcal{E}_{2Q}^{(\mathcal{P})}$ Rayleigh Ritz variational estimates obtained, as well as the E parameter value, E^*, for which the smallest RR Hamiltonian expectation value is observed ($\mathrm{Min}_E \mathcal{E}_{2Q}^{(\mathcal{P})}(E) \equiv \mathcal{E}_{2Q}^{(\mathcal{P})}(E^*)$).

For $g = 1$, in all three cases $Q = 2, 3, 4$, corresponding to the quartic, sextic, and octic potentials, respectively, the ensuing x-configuration space RR analysis did not yield converging bounds to the true ground-state energy value cited in the last column of table 1. The numerical results (not presented here in their entirety) reveal that as the order, $\mathcal{P}$, of the calculation increases, the RR estimates significantly diverge from the true physical values. This behaviour is contrary to the moment equation RR variational analysis where each increase in the order of the calculation yielded better results.

The quartic anharmonic oscillator results were consistent with the true value. Thus for $\mathcal{P} = 4$, we have $\mathcal{E}_4^{(4)} = 1.392\,479$ ($E^* = 1.3852$); however, as the order increases, the results appear to diverge from the true value of 1.392 351 642. Specifically, $\mathcal{E}_4^{(5)} = 1.392\,59$ ($E^* = 1.3964$).

For the sextic and octic potentials, the results were dramatically inferior, becoming progressively worse as $\mathcal{P}$ increased. Thus, for the sextic case we obtained $\mathcal{E}_6^{(2)} \approx 1.443$ ($E^* = 1.5691$), whereas $\mathcal{E}_6^{(7)} \approx 1.813\,61$ ($E^* = 1.435\,25$). For the octic anharmonic potential, $\mathcal{E}_8^{(2)} \approx 1.5516$ at $E^* = 1.6116$, whereas $\mathcal{E}_8^{(4)} \approx 2.3332$ at $E^* = 1.1535$.

The preceding configuration space results substantiate the earlier remarks that such local expansions are insensitive to the global nature of eigenenergy quantization. Of course, one could make some adjustments to improve the situation (i.e. treat the exponent variationally); however, our objetive is to contrast the relative effectiveness of the moment equation representation RR analysis compared to an analogous, but unsuccessfull, configuration space implementation.

4. A rational fraction potential

Although the examples presented were faciliated by the polynomial nature of the configuration space potential, there is nothing in the preceding formalism that limits its applicability to other types of potentials. Thus, one can examine the potential problem

$$V(x) = x^2 + \frac{\lambda x^2}{1 + gx^2} .$$

Upon multiplying both sides of the corresponding Schrödinger equation by $1 + gx^2$, multiplying by x^{2p}, and integrating, one obtains a moment equation of the form

$$
\begin{aligned}
gu(p+2) = {} & [gE - \lambda - 1]u(p+1) + [E + 2g(p+1)(2p+1)]u(p) \\
& + 2p(2p-1)u(p-1) \qquad p \geqslant 0
\end{aligned}
\tag{4.1}
$$

for the even order Hamburger moments of the ground-state wavefunction, $u(p) = \int_{-\infty}^{\infty} \mathrm{d}x\, x^{2p}\Psi(x)$.

The moment equation is of missing moment order 1. Accordingly, we can take $u(p) = \sum_{l=0}^{1} \mathcal{M}_E(p,l)u(l)$, where the $\mathcal{M}_E(p,l)$ coefficients satisfy equation (4.1), with respect to the 'p' index, and obey the initialization conditions $\mathcal{M}_E(i,j) = \delta_{i,j}$, for $0 \leqslant i, j \leqslant 1$. We may then express the formal Fourier transform of the wavefunction by

$$
\tilde{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \sum_{p=0} \frac{(-\mathrm{i}k)^{2p}}{(2p)!} u(p) \qquad \text{or} \qquad \tilde{\Psi}(k) = \sum_{l=0}^{1} u(l)\tilde{\mathcal{T}}_l(E,k)
$$

as before. A simple asymptotic analysis should confirm that the functions

$$
\tilde{\mathcal{T}}_l(E,k) = \frac{1}{\sqrt{2\pi}} \sum_{p=0} \frac{(-\mathrm{i}k)^{2p}}{(2p)!} \mathcal{M}_E(p,l)
$$

have an infinite radius of convergence in k-space.

The Fourier space representation for the Schrödinger equation (i.e. $[-\partial^2 + V(x)]\Psi = E\Psi$) is

$$
[k^2 - \partial_k^2]\tilde{\Psi}(k) - \frac{\lambda}{\sqrt{2\pi}} \partial_k^2 \int \mathrm{d}k_1\, \tilde{\mathcal{R}}(k-k_1)\tilde{\Psi}(k_1) = E\tilde{\Psi}(k) \tag{4.2}
$$

where $\tilde{\mathcal{R}}(k)$ is the Fourier transform of $1/(1+gx^2)$ or $\tilde{\mathcal{R}}(k) = \sqrt{\pi/2g}\exp(-|k|/\sqrt{g})$; however, we will not need to work explicitly in Fourier space.

The energy expectation value

$$
\mathcal{E}(E, u(0), u(1)) = \frac{\langle\tilde{\Psi}(k)|\tilde{\mathcal{H}}|\tilde{\Psi}(k)\rangle}{\langle\tilde{\Psi}(k)|\tilde{\Psi}(k)\rangle} \tag{4.3}
$$

can be approximated by $\tilde{\Psi}(k) = \exp(\frac{1}{2}k^2)\sum_{l=0}^{1} u(l)\mathcal{C}^{(l)}(k)$, and $\mathcal{C}^{(l)}(k) \equiv \exp(-\frac{1}{2}k^2)\tilde{\mathcal{T}}_l(E,k) \approx \sum_{p=0}^{\mathcal{P}} C_p^{(l)}(-\mathrm{i}k)^{2p}$, as was done for the anharmonic potentials. The $C_p^{(l)}$ coefficients satisfy

$$
C_p^{(l)} = \frac{1}{\sqrt{2\pi}} \frac{\mathcal{M}_E(p,l)}{(2p)!} - \sum_{k=0}^{p-1} \frac{(\frac{1}{2})^{p-k}}{(p-k)!} C_k^{(l)}.
$$

We can perform all the necessary integrals in configuration space. Simply replace $\Psi(x) \to \sum_{l=0}^{1} u(l) \sum_{p=0}^{\mathcal{P}} C_p^{(l)} \partial_x^{2p} \exp(-x^2/2)$. Note that unlike the anharmonic cases previously considered, we choose the exponential argument to be $-x^2/2$, not $-x^2$. For this problem, the former yields the excellent results quoted below.

Let us define $F^Q(x) \equiv \partial_x^Q \exp(-x^2/2)$. If Q is even, let $j = Q/2$ and $\delta_Q \equiv 0$. If Q is odd, $j = (Q-1)/2$ and $\delta_Q \equiv 1$. We then have

$$F_Q(x) = \exp(-x^2/2)\ Q!\ \sum_{p=0}^{j} \frac{(-x)^{2p+\delta_Q}}{(2p+\delta_Q)!} \frac{(-\frac{1}{2})^{j-p}}{(j-p)!}\,. \tag{4.4}$$

The expectation value becomes (to order $\mathcal{P}$)

$$\mathcal{E}(E, u(0), u(1)) = \frac{\sum_{l_1,l_2=0}^{1} u(l_1)\mathcal{N}(l_1,l_2)u(l_2)}{\sum_{l_1,l_2=0}^{1} u(l_1)\mathcal{D}(l_1,l_2)u(l_2)} \tag{4.5}$$

where

$$\mathcal{N}(l_1,l_2) = \sum_{j_1,j_2=0}^{\mathcal{P}} C_{j_1}^{(l_1)} \left(\int \mathrm{d}x\ F_{2j_1}(x) \left[-\partial_x^2 + x^2 + \frac{\lambda x^2}{(1+gx^2)} \right] F_{2j_2}(x) \right) C_{j_2}^{(l_2)} \tag{4.6a}$$

(note that the $\int \mathrm{d}x\ F_{2j_1}(-\partial_x^2)F_{2j_2}$ term is equivalent to $\int \mathrm{d}x\ F_{2j_1+1}F_{2j_2+1}$) and

$$\mathcal{D}(l_1,l_2) = \sum_{j_1,j_2=0}^{\mathcal{P}} C_{j_1}^{(l_1)} \left(\int \mathrm{d}x\ F_{2j_1}(x) F_{2j_2}(x) \right) C_{j_2}^{(l_2)}\,. \tag{4.6b}$$

The integrals appearing in equations (4.6*a*), (4.6*b*) can be readily done through standard integration routines. Note that these integrals only need to be done once, they are independent of the E parameter (recall that the $C_j^{(l)}$ coefficients are implicitly E dependent).

Table 2. Moment equation RR analysis, $V(x) = x^2 + \lambda x^2/(1+gx^2)$, $g = 2$, $\lambda = 0.1$.

$\mathcal{P}$	E^*	$\mathcal{E}^*$	Other methods
2	1.026	1.017 181 806	1.017 176 $< E_0 <$ 1.017 185[a]
3	1.020	1.017 181 063	1.017 281 60[b]
4	1.0181	1.017 180 708	1.017 180 290 061 535 662 051 677 19[c]
5	1.0176	1.017 180 531	

[a] Handy (1985).
[b] Lai-Lin (1982).
[c] Hodgson (1988).

The results of our Rayleigh–Ritz variational analysis with respect to the two-dimensional matrices appearing in (4.6*a*), (4.6*b*), for arbitrary $\mathcal{P} \leqslant 5$ are given in table 2. We picked the parameter values $g = 2$ and $\lambda = 0.1$, the subject of some modest controversy (Handy 1985) in contrasting the eigenvalue moment method (EMM) of Handy and Bessis (1985) with the Hellman–Feynman hypervirial variational approach of Lai and Lin (1982) (LL). The latter method yielded the ground-state energy estimate of $E_0^{(\mathrm{LL})} = 1.017\,281\,60$. The EMM analysis gave the bounds $1.017\,176 < E_0 < 1.017\,185$, clearly invalidating the implied accuracy of the LL results. The accuracy of the EMM bounds was confirmed subsequently by Hodgson (1988).

The aforementioned EMM bounds were generated not with respects to the moment equation in (4.1) but with respects to a more suitable transformation of it into another function-representation space (Handy 1985). Direct application of EMM theory to the moment equation in (4.1) yields poor bounds: $0.49 < E_0 < 1.60$, for an expansion order of $\mathcal{P} = 30$. Despite this, the moment equation Rayleigh Ritz analysis based on (4.1) gives excellent results surpassing the quoted EMM bounds. These are given in table 2.

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