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# Generating bounds for the discrete state energy values of the infinite quantum lens potential

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## Abstract

Moment based methods have produced efficient multiscale quantization algorithms for solving singular perturbation/strong coupling problems. One of these, the eigenvalue moment method (EMM), developed by Handy and Bessis (Handy C R and Bessis D 1985 *Phys. Rev. Lett.* **55** 931) and Handy *et al* (Handy C R, Bessis D, Sigismondi G and Morley T D 1988b *Phys. Rev. Lett.* **60** 253), generates converging lower and upper bounds to a specific discrete state energy, once the signature property of the associated wavefunction is known. This method is particularly effective for multi-dimensional, bosonic ground state problems, since the corresponding wavefunction must be of uniform signature, and can be taken to be positive. Despite this, the vast majority of problems studied have been on unbounded domains. The important problem of an electron in an infinite quantum lens potential defines a challenging extension of EMM to systems defined on a compact domain. We investigate this in this paper, and introduce novel modifications to the conventional EMM formalism that facilitate its adaptability to the required boundary conditions.

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## 1. Introduction

Self-assembled quantum dots (QDs), obtained by interrupted growth in strained semiconductors, offer an attractive and fascinating array of physical properties (Leonard *et al* 1993, 1994). Differential capacitance (Drexler *et al* 1994, Miller *et al* 1997), magnetic-conductance (Medeiros-Ribeiro *et al* 1997), and optical experiments (Fafard *et al* 1994, Lee *et al* 2000) demonstrate that electronic states are strongly confined inside such structures.

Typically, a lens geometry is assumed (Leonard *et al* 1994), with a circular cross section of maximum radius  $a$ , and maximum thickness  $b$ ; wherein the charge carriers are confined by a hard wall (infinite) potential (refer to figure 1). The mathematical characterization of the

energy levels of such nanostructures is a delicate problem, particularly in the thin lens limit  $\frac{b}{a} \rightarrow 0$ , which corresponds to a singular perturbation regime.

Recently, conformal analysis methods were used to solve the infinite quantum lens potential (Rodriguez *et al* 2001). Preliminary results underscore the delicate nature of the thin lens regime. In order to better assess the accuracy of such methods, we have developed an eigenenergy bounding procedure that, at low order, yields exceptionally tight bounds to the discrete state energy levels. The details are presented here, with respect to the lowest energy state within each azimuthal quantum number subspace.

Our bounding procedure is based on the eigenvalue moment method (EMM) formalism of Handy *et al* (1985, 1988a, 1988b). This, linear programming based (Chvatal 1983) formalism has been shown to be exceptionally well suited for singular perturbation/strong coupling problems. It is straightforward to use, and involves the application of fundamental theorems arising from the classic *moment problem* (Shohat and Tamarkin 1963, Akhiezer 1965), as well as theorems pertaining to the signature structure of bosonic (ground state) wavefunctions (Reed and Simon 1978).

The *moment problem* deals with the necessary and sufficient properties that the moments of a function must satisfy in order for the function to be non-negative. Additional questions of uniqueness arise; however, within the context of EMM, the uniqueness of the physical solution, as implicitly incorporated within the necessary moment relations considered, circumvents these concerns.

In the following subsections we outline the essentials, first for the multi-dimensional  $\text{Re}^3$ -EMM formulation, and then for a compact domain,  $\mathcal{D} \subset \text{Re}^3$ .

In generating the necessary moment equation (ME) for the compact domain case (i.e. transforming the Schrödinger equation into an equation for the relevant power moments), boundary terms will appear. These boundary terms will correspond to generalized moments of reduced dimension due to integrating along the boundary of  $\mathcal{D}$ . One prefers an ME formulation devoid of such complicating expressions. An additional novel contribution of this work is the development of an EMM prescription for eliminating the boundary terms from the relevant ME representation.

This is not trivial. In the appendix we present several one-dimensional examples demonstrating the pitfalls that can ensue if things are not done properly. The reader may wish to consult these examples first. We also include in the appendix a review of EMM, in one dimension, for the sake of a self-contained presentation.

We close this section by emphasizing that EMM can be characterized as an affine map invariant variational procedure. We believe that this explains the robustness of the method, and its suitability for addressing singular perturbation type problems where sensitivity to multiscale features of a problem are important. In sections 2–4 we discuss the specifics of the EMM analysis as applied to the infinite quantum lens potential.

### 1.1. EMM on $\text{Re}^3$

The multi-dimensional bosonic ground state wavefunction must be of uniform signature, which can be taken to be non-negative (Reed and Simon 1978):

$$\Psi_{gr}(\vec{r}) \geq 0. \quad (1)$$

It will then satisfy the positive integral relations:

$$\iiint dx dy dz (\mathcal{P}_C(\vec{r}))^2 \Psi_{gr}(\vec{r}) > 0 \quad (2)$$

where  $\mathcal{P}_C \equiv \sum_{l,m,n} C_{l,m,n} x^l y^m z^n$  is an arbitrary polynomial. In terms of the power moments,

$$\mu(\vec{p}) \equiv \iiint dx dy dz x^{p_1} y^{p_2} z^{p_3} \Psi_{gr}(\vec{r}) \tag{3}$$

for non-negative integer values,  $\vec{p} = (p_1, p_2, p_3)$ ,  $p_i \geq 0$ , the integrals in equation (2) become the Hankel–Hadamard (HH), quadratic form, inequalities:

$$\sum_{l_1, m_1, n_1} \sum_{l_2, m_2, n_2} C_{l_1, m_1, n_1} \mu(l_1 + l_2, m_1 + m_2, n_1 + n_2) C_{l_2, m_2, n_2} > 0 \tag{4}$$

for arbitrary  $C$ 's (not all identically zero).

The Fourier transform of the  $L^2$  Schrödinger equation solutions, usually admits a power series expansion, whose Taylor coefficients (i.e. the moments) satisfy a linear recursion relation. This is referred to as the moment equation (ME). Although implicitly derived for the physical solutions, the ME relation can be extended into the energy space domain, and thus exists for any energy parameter value,  $E$ .

The entire set of power moments is divided into two subsets:

$$\{\mu(\vec{p}) | \vec{p} \geq \vec{0}\} = \{\mu(\vec{\ell}) | \vec{\ell} \in \mathcal{M}_s\} \cup \{\mu(\vec{p}) | \vec{p} \notin \mathcal{M}_s\}. \tag{5}$$

The first subset corresponds to the initialization moments, or *missing moments*, which must be specified before all of the other moments can be generated through the ME relation.

The generated moments, those in the second subset, are linearly dependent on the missing moments. We can represent the ME relationship as

$$\mu(\vec{p}) = \sum_{\vec{\ell} \in \mathcal{M}_s} M_E(\vec{p}, \vec{\ell}) \mu(\vec{\ell}) \tag{6}$$

$\vec{p} \notin \mathcal{M}_s$ . We emphasize that the  $\vec{\ell}$  index notation exclusively refers to the missing moment variables.

The  $M_E$  coefficients are dependent on  $E$ , and can be defined so that the above is also valid for the missing moments as well (i.e.  $M_E(\vec{\ell}_1, \vec{\ell}_2) = \delta_{\vec{\ell}_1, \vec{\ell}_2}$ , for  $\vec{\ell}_{1,2} \in \mathcal{M}_s$ ).

For 1-space dimension systems, the number of missing moments is finite, and denoted by  $1 + m_s$ . For multi-dimensional systems,  $\text{Re}^{d \geq 2}$ , the number of missing moments is infinite; however, the set of missing moments naturally decomposes into a hierarchy of finite-dimensional subspaces:

$$\{\mu(\vec{\ell}) | \vec{\ell} \in \mathcal{M}_s\} = \dots \mathcal{U}_\infty \dots \supset \mathcal{U}_n \supset \mathcal{U}_{n-1} \dots \supset \mathcal{U}_1 \tag{7}$$

where we implicitly assume that the missing moment variables are sequentially indexed, in some convenient manner, and  $\mathcal{U}_n$  denotes the missing moment subspace consisting of the first  $n$  missing moments.

Each of the missing moment finite-dimensional subspaces,  $\mathcal{U}_n$ , determines a finite set of generated moments.

Since the ME is a homogeneous relation, one must impose a normalization condition. This is normally done with respect to the missing moments. For instance, we can take

$$\sum_{\vec{\ell} \in \mathcal{U}_n} \mu(\vec{\ell}) = 1. \tag{8}$$

Adopting this, one then substitutes the ME relation (equation (6)) into the HH inequalities (equation (4)). Since all the moments are linear in the missing moments, a linear programming problem is defined of the form

$$\sum_{\vec{\ell}} \Lambda_{\vec{\ell}}(E; C) \mu(\vec{\ell}) > 0 \tag{9}$$

where the  $\Lambda$  coefficients are nonlinearly dependent on  $E$ , and quadratically dependent on the (arbitrary)  $C$ 's.

In implementing EMM, we must first define an appropriate enumeration for all of the non-negative 3-tuple integer vectors,  $\{(l, m, n) | l, m, n \geq 0\}$ . Assuming this (i.e.  $(l, m, n)_i$ ), we then have

$$\{(l, m, n) | l, m, n \geq 0\} = \mathcal{T}_\infty \cdots \supset \mathcal{T}_i \supset \mathcal{T}_{i-1} \cdots \supset \mathcal{T}_1 \tag{10}$$

where  $\mathcal{T}_i$  denotes the set of 3-tuple integer vectors containing the first  $i$  vectors. We do not have to work with the  $\mathcal{T}_i$ 's sequentially. We can pick any subsequence of this. Let  $i \rightarrow I$ .

Restrict the  $\mathcal{P}_C$  polynomials to those whose monomial terms have degrees lying within  $\mathcal{T}_I$ . From equation (4) it becomes clear that the required ('generated') moments are  $\{\mu(\vec{p}) | \vec{p} = (l_1, m_1, n_1) + (l_2, m_2, n_2), \text{ where } (l_{1,2}, m_{1,2}, n_{1,2}) \in \mathcal{T}_I\}$ . One must then determine the missing moment subsets,  $\mathcal{U}^{(I)} \equiv \mathcal{U}_{n(I)}$ , that generate these. They in turn define the linear programming (HH-inequality) problem symbolized in equation (9).

For a given dimension,  $I$ , at an arbitrary energy value,  $E$ , the HH linear inequalities will either have a missing moment solution set,  $\mathcal{U}_E^{(I)}$ , or not  $\mathcal{U}_E^{(I)} = \emptyset$ . If there is a solution set, it must be convex. This convex set may be considered as the intersection of an (uncountably) infinite number of polytopes (convex sets formed from the intersection of a finite number of hyperplanes).

The objective of the linear programming based, algorithmic implementation of EMM, is to quickly determine the existence or nonexistence of  $\mathcal{U}_E^{(I)}$ . At any order  $I$ , the feasible energy values (those for which the convex set exists) define an energy interval,  $(E_L^{(I)}, E_U^{(I)})$ , within which the true ground state value,  $E_{gr}$ , must lie. As the order is increased, the energy endpoints define converging lower and upper bounds to  $E_{gr}$ :

$$E_L^{(I)} \leq E_L^{(I+1)} \leq \dots < E_{gr} < \dots \leq E_U^{(I+1)} \leq E_U^{(I)} \quad I \rightarrow \infty. \tag{11}$$

### 1.2. EMM on $\mathcal{D} \subset \text{Re}^3$

When EMM is to be implemented on a subset,  $\mathcal{D}$ , of the full space, one must consider more moment constraints than those in equations (2) or (4). We want

$$\Psi(\vec{r}) = 0 \quad \text{for } \vec{r} \in \overline{\mathcal{D}} \tag{12}$$

where  $\overline{\mathcal{D}}$  denotes the complement of the set. We need to define moment problem constraints that insure the conditions in equation (12).

Define the decomposition

$$\overline{\mathcal{D}} = \bigcup_{j=1}^J \Omega_j \tag{13}$$

where  $\Omega_j \cap \mathcal{D} = \emptyset$ . Assume that there exist polynomials,  $\mathcal{P}_{\Omega_j}(\vec{r})$ , with the properties

$$\mathcal{P}_{\Omega_j}(\vec{r}) \text{ is } \begin{cases} \geq 0 & \vec{r} \in \text{Re}^3 - \Omega_j \\ < 0 & \vec{r} \in \Omega_j. \end{cases} \tag{14}$$

Then, for each of these polynomials, we supplement equations (2), (4) by

$$\iiint_{\mathcal{D}} dx dy dz (\mathcal{P}_C(\vec{r}))^2 \mathcal{P}_{\Omega_j}(\vec{r}) \Psi_{gr}(\vec{r}) > 0. \tag{15}$$

We can motivate this as follows. The inequalities in equation (2) only yield that  $\Psi_{gr}$  is non-negative over  $\text{Re}^3$ . Each of the additional inequalities in equation (15) tells us that  $\mathcal{P}_{\Omega_j} \Psi_{gr}$  is also non-negative on  $\text{Re}^3$ , if we replace the integration domain  $\mathcal{D}$  by  $\text{Re}^3$  in equation (15). However,  $\Psi_{gr}$  and  $\mathcal{P}_{\Omega_j} \Psi_{gr}$  cannot be non-negative on  $\Omega_j$  without  $\Psi_{gr}$  being zero over  $\Omega_j$ .

Thus, if we had replaced  $\mathcal{D} \rightarrow \text{Re}^3$  in equation (15), we would conclude that equation (12) holds, thereby justifying the restriction of equation (15) to the  $\mathcal{D}$  domain, as explicitly noted.

The zeros of any multi-dimensional polynomial do not necessarily correspond to the boundary of a convex set. Thus, in principle, the domain  $\mathcal{D}$  can be nonconvex, although the particular problem being considered here corresponds to a convex domain.

### 1.3. Removing the boundary terms in the moment equation

In deriving the ME relation for the moments restricted to  $\mathcal{D}$ , boundary terms are introduced. We prefer, where possible, to remove these, since they complicate (although not necessarily prevent) the implementation of EMM. To motivate our approach, we consider the case of a free particle restricted to a compact domain (i.e. the potential becomes infinite on  $\overline{\mathcal{D}}$ ):

$$-\nabla^2 \Psi(\vec{r}) = E \Psi(\vec{r}) \quad (16)$$

for  $\vec{r} \in \mathcal{D}$ , and  $\Psi = 0$ , on the boundary.

Consider any function,  $G(\vec{r})$ , and multiply both sides of the above, followed by the appropriate ‘integration by parts’ differential operator rearrangements. We obtain

$$-(\vec{\nabla}(G\vec{\nabla}\Psi) - \vec{\nabla}(\Psi\vec{\nabla}G) + \Psi\nabla^2G) = E G\Psi. \quad (17)$$

If  $G = 0$  on the boundary of  $\mathcal{D}$  (and on which  $\Psi = 0$ , also) then upon integrating equation (17) over  $\mathcal{D}$ , no surface terms appear:

$$-\iiint_{\mathcal{D}} d^3r \Psi \nabla^2 G = E \iiint_{\mathcal{D}} d^3r \Psi G. \quad (18)$$

We can take  $G = x^l y^m z^n \mathcal{P}_z(\vec{r})$ , where the polynomial  $\mathcal{P}_z(\vec{r})$  becomes zero on the boundary of  $\mathcal{D}$  (the intended connotation of the  $z$  subscript). For reasons clarified below,  $\mathcal{P}_z$  must not have any zeros within  $\mathcal{D}$ . Upon varying  $l, m, n$ , there ensues a ME for the moments of  $\Psi$ .

If we allow  $\mathcal{P}_z$  to have zeros within  $\mathcal{D}$ , then the resulting ME does not uniquely correspond to the physical system of interest, and EMM will fail to generate any bounds.

To clarify this important point, assume that  $\mathcal{P}_z(\vec{r}_z) = 0$ , corresponds to a zero within  $\mathcal{D}$ . Then the modified equation

$$-\nabla^2 \Psi(\vec{r}) = E \Psi(\vec{r}) + \mathcal{A} \delta(\vec{r} - \vec{r}_z), \quad (19)$$

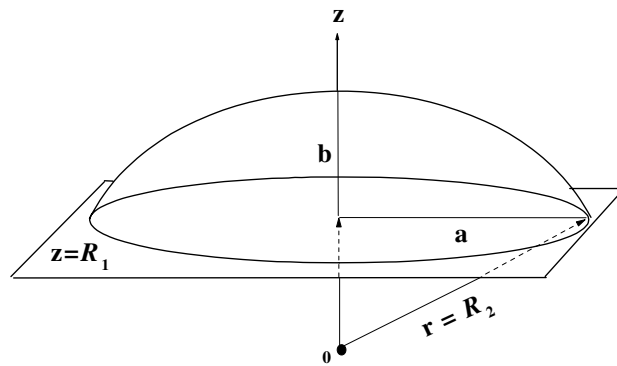
for arbitrary  $\mathcal{A}$ , will also transform into equation (17). Since for each  $\mathcal{A}$  there may be a non-negative solution, one cannot expect that application of EMM, to the ME derived from equation (17), will yield a unique  $E$  value. That is, no converging bounds should result.

In the appendix, in addition to the pedagogic review of EMM in 1-dimension (i.e. appendix A), we also show some of the consequences of incorrectly specifying  $\mathcal{P}_z$  (i.e. appendix B).

### 1.4. EMM: an affine map invariant variational procedure

The EMM formalism has been used to generate rapidly converging bounds to the ground state binding energy of hydrogenic atoms in superstrong magnetic fields (Handy *et al* 1988a, b), otherwise known as the *quadratic Zeeman effect*. This problem had been notoriously difficult, yielding varying results depending on the method used. The ability of EMM to define tight bounds to the ground state binding energy enabled one to discriminate between competing (energy estimation) methods. In particular, it confirmed the results of LeGuillou and Zinn-Justin (1983), which were based on order dependent, conformal analysis.

The consistency of the EMM generated results, and those based on LeGuillou and Zinn-Justin’s conformal analysis, is more than a coincidence. In one dimension, an affine map



**Figure 1.** Quantum lens geometry of height  $b$  and circular cross section of radius  $a$ .

transformation of the point  $x$  is defined by  $x \rightarrow \frac{x-\tau}{s}$ , where  $s$  and  $\tau$  are scale and translation parameters, respectively. An affine map transform of a given function,  $\mathcal{P}(x) \rightarrow \mathcal{P}(\frac{x-\tau}{s})$ , corresponds to a translation and stretching (or contraction).

The variational procedure inherent to EMM, is, in fact, affine map invariant. This is immediately clear from equation (2), since the variation samples over all polynomial functions; however, the space of polynomials is invariant under affine transforms. To this extent, EMM is in keeping with the underlying philosophy of conformal analysis, and should yield either consistent, or better, results.

This affine map invariance underscores the fundamental complementarity between moment quantization methods, such as EMM, and explicitly multiscale methods such as wavelet transform theory (Handy and Murenzi 1998). This further confirms the relevancy of EMM to singular perturbation type problems which require a careful balancing between large and small scale contributions.

Despite the numerous types of problems the EMM formalism has been applied to, as reviewed in the cited references, it has not been used on problems defined on a compact domain. Such problems require a modification of the basic formalism, in order to adapt them to the required boundary conditions, as previously discussed. The infinite quantum lens potential is one such important case, to which we now turn.

## 2. The infinite quantum lens problem

The quantum lens geometry, as shown in figure 1, is bounded by the  $z = R_1$  plane, and the sphere of radius  $R_2$ :

$$\text{Lens domain} = \{z \geq R_1\} \cap \{r \leq R_2\} \quad (20)$$

where  $R_1 < R_2$ .

In a cylindrical coordinate representation, the Schrödinger equation for the infinite quantum lens potential problem becomes (in energy units  $E_0 = \frac{\hbar^2}{2ma^2}$ , and length in units of the radius,  $a = \sqrt{R_2^2 - R_1^2}$ ):

$$-\left(\frac{1}{\rho}\partial_\rho(\rho\partial_\rho\Psi) + \frac{1}{\rho^2}\partial_\phi^2\Psi + \partial_z^2\Psi\right) = E\Psi(\rho, \phi, z) \quad (21)$$

where ( $r^2 = \rho^2 + z^2$ , note that we will be working with the  $r^2$  and  $z^2$  coordinates)

$$R_1^2 \leq r^2 \leq R_2^2 \quad \text{and} \quad R_1^2 \leq z^2 \leq r^2 \tag{22}$$

for  $z > 0$ . The boundary condition on the wavefunction is

$$\Psi(\rho, \phi, z) = \begin{cases} 0 & z^2 = R_1^2 \\ 0 & r^2 = R_2^2. \end{cases} \tag{23}$$

The radii  $R_1$  and  $R_2$  can be redefined in terms of the quantum lens parameters  $a$  and  $b$ , where

$$a^2 = R_2^2 - R_1^2 \quad \text{and} \quad b = R_2 - R_1 \tag{24}$$

or, alternatively,

$$R_2 = \frac{a^2 + b^2}{2b} \quad \text{and} \quad R_1 = \frac{a^2 - b^2}{2b}. \tag{25}$$

The lens domain transforms into a triangular domain in the  $\{r^2, z^2\}$  coordinate space, or, equivalently,

$$\omega \equiv R_2^2 - r^2 \quad \text{and} \quad v = z^2 - R_1^2. \tag{26}$$

The corresponding domain is

$$0 \leq \omega \leq a^2 \quad \text{and} \quad 0 \leq v \leq a^2 - \omega. \tag{27}$$

Equation (21) is axially symmetric, and the solutions assume the form  $\Psi(\rho, \phi, z) = e^{-im\phi}\psi(\rho, z)$ .

In the  $\{\omega, v\}$  coordinate system, the Schrödinger equation becomes (i.e. first transforms into  $\{\rho^2, z^2\}$  coordinates, then into  $\{r^2, z^2\}$ , and finally into  $\{\omega, v\}$ ):

$$-4((R_2^2 - \omega)\partial_\omega^2 - \frac{3}{2}\partial_\omega - 2(R_1^2 + v)\partial_\omega\partial_v + \frac{1}{2}\partial_v + (R_1^2 + v)\partial_v^2)\psi(\omega, v) + \frac{m^2}{a^2 - \omega - v}\psi(\omega, v) = E\psi(\omega, v). \tag{28}$$

The boundaries  $r^2 = R_2^2$  and  $z^2 = R_1^2$  become  $\omega = 0$  and  $v = 0$ . According to equation (27), the  $\{\omega, v\}$  physical domain is restricted to the lower left triangle of the  $[0, a^2] \times [0, a^2]$  square region. The hypotenuse of this triangle corresponds to  $a^2 - \omega - v = \rho^2 = 0$ . The wavefunction is not zero along it; although it is zero along  $\omega = 0$  and  $v = 0$ .

Although we shall work within the  $\{\omega, v\}$  coordinates, in order to derive the necessary MEs, we note that we can rewrite the above equation in terms of the coordinates  $\xi \equiv \omega + v$  and  $\eta = \omega - v$ . The derivatives become  $\partial_\omega = \partial_\xi + \partial_\eta$ ,  $\partial_v = \partial_\xi - \partial_\eta$ . The  $\rho = 0$  boundary corresponds to  $\xi = a^2$ . In terms of these new coordinates, the Schrödinger equation becomes

$$-4([a^2 - \xi]\partial_\xi^2 + 2[a^2 - \xi]\partial_\xi\partial_\eta + [R_2^2 + 3R_1^2 + (\xi - 2\eta)]\partial_\eta^2 - \partial_\xi - 2\partial_\eta)\psi + \frac{m^2}{a^2 - \xi}\psi = E\psi. \tag{29}$$

We shall refer to the various function coefficients of the derivative operators in equation (29) (i.e.  $\sum_{i,j} C_{i,j}\partial_\xi^i\partial_\eta^j$ ) by

$$C_{i,j}(\xi, \eta) = \begin{cases} a^2 - \xi & i = 2 \quad j = 0 \\ 2[a^2 - \xi] & i = 1 \quad j = 1 \\ R_2^2 + 3R_1^2 + (\xi - 2\eta) & i = 0 \quad j = 2 \\ -1 & i = 1 \quad j = 0 \\ -2 & i = 0 \quad j = 1. \end{cases} \tag{30}$$

Our objective is to derive, for a given quantum number  $m$ , a ME for equation (28), involving the moments

$$u(p, q) \equiv \int_0^{a^2} d\omega \int_0^{a^2-\omega} dv \omega^p v^q \psi(\omega, v) \tag{31}$$

and no boundary terms.



In order to achieve the above, for the  $m = 0$  case, we will have to multiply both sides of equation (28) by  $G(\omega, \nu) = \omega^p \nu^q$ , where  $p, q \geq 1$ . We note that  $G(\omega, \nu) = 0$ , along both boundaries  $\omega = 0$  and  $\nu = 0$ , where  $\psi = 0$ . Integrating over the triangular domain in  $\{\omega, \nu\}$  does not introduce any boundary terms at all, not even along the  $\rho = 0$  boundary, where  $\psi \neq 0$ . We prove this (with respect to the representation in equation (29)), below, for each of the contributing terms in the ME relation.

- (i) The terms  $G(\omega, \nu)C_{0,2}(\xi, \eta)\partial_\eta^2\psi$  and  $G(\omega, \nu)C_{0,1}(\xi, \eta)\partial_\eta\psi$ , do not introduce any boundary terms since those generated by integration by parts (in the  $\eta$  direction) correspond to points where  $G(\omega, \nu) = 0$  and  $\psi = 0$ .
- (ii) The integration by parts of  $G(\omega, \nu)C_{1,1}(\xi, \eta)\partial_\xi\partial_\eta\psi$  reduces to

$$\partial_\xi(GC_{1,1}\partial_\eta\psi) - \partial_\eta(\psi\partial_\xi(GC_{1,1})) + \psi\partial_\xi\partial_\eta(GC_{1,1}). \quad (32)$$

The boundary terms produced by the first term (along the  $\xi$  direction) are zero since at one point (corresponding to either  $\omega = 0$  or  $\nu = 0$ ) we have  $G(\omega, \nu) = 0$ , while at the other (corresponding to  $\xi = a^2$ ), we have  $C_{1,1} = 0$ . The boundary terms from the second term are also zero, since at both ends (along the  $\eta$  direction) we have  $\psi = 0$ .

- (iii) The integration by parts for  $G(\omega, \nu)[C_{2,0}(\xi, \eta)\partial_\xi^2\psi - \partial_\xi\psi]$  gives us

$$\partial_\xi(GC_{2,0}\partial_\xi\psi) - \partial_\xi(\psi\partial_\xi(GC_{2,0})) - \partial_\xi(G\psi) + [\partial_\xi^2(GC_{2,0}) + \partial_\xi G]\psi. \quad (33)$$

The first term introduces no boundary terms (along the  $\xi$  direction) because at one endpoint we have  $G(\omega, \nu) = 0$ , while at the other  $C_{2,0} = 0$ . The second and third terms have no boundary term at the point corresponding to  $\psi = 0$ . However, at  $\xi = a^2$ , since  $\partial_\xi C_{2,0} = -1$ , we obtain a cancellation between the only surviving boundary terms. This concludes the proof that no boundary terms arise for the  $m = 0$  case.

For the  $m \neq 0$  case, we have that  $\Psi = 0$  for  $\rho = a^2 - \omega - \nu = 0$  (refer to section 4). Thus, one would think that the choice of  $G(\omega, \nu) = \omega^p \nu^q (a^2 - \omega - \nu)$ , for  $p, q \geq 1$ , would lead to an acceptable ME. For such a selection, the preceding argument still holds, although the final cancellation of both boundary terms is unnecessary because of the additional  $\rho^2 = (a^2 - \xi)$  factor introduced through the modified  $G$ . However, a careful review of the boundary term cancellation analysis presented, shows that nowhere do we explicitly make use of  $\Psi(\rho = 0, z) = 0$ . Thus, the ensuing ME obtained from  $G(\omega, \nu) = \omega^p \nu^q (a^2 - \omega - \nu)$ , cannot uniquely correspond to the physical system in question. That is, the generated ME would correspond to equation (21) plus the introduction of additional  $\delta(\rho)$ -like inhomogeneous terms.

This is an important point that deserves repetition. Thus, not only must  $G$  be zero along the boundary,  $\partial\mathcal{D}$ , but also  $\psi$  must be zero on  $\partial\mathcal{D}$ , and this must explicitly contribute in the elimination of the boundary terms.

Thus an alternate formulation is required for the  $m \neq 0$  case. Fortunately, a very simple modification allows us to address this case. This is discussed in section 4.

### 3. The $m = 0$ moment equation

The ME for the  $m = 0$  case is

$$\begin{aligned} -\frac{E}{4}u(p, q) &= R_2^2 p(p-1)u(p-2, q) - \left[ p^2 + \frac{3p}{2} + 2pq \right] u(p-1, q) \\ &\quad - 2R_1^2 pq u(p-1, q-1) + \left[ q^2 + \frac{q}{2} \right] u(p, q-1) + R_1^2 q(q-1)u(p, q-2) \\ &\quad \text{for } p, q \geq 1. \end{aligned} \quad (34)$$

The *missing moments*  $\{u(0, 0), \dots, u(N, 0)\}$  and  $\{u(0, 1), \dots, u(0, N)\}$ , generate all the moments within the square grid  $[0, N] \times [0, N]$ . We can index the missing moments according to  $\chi_0 \equiv u(0, 0), \chi_1 \equiv u(1, 0), \dots, \chi_N \equiv u(N, 0), \chi_{N+1} \equiv u(0, 1), \dots, \chi_{2N} \equiv u(0, N)$ .

We can then determine the energy dependent coefficients linking the moments to the missing moments

$$u(p, q) = \sum_{\ell=0}^{m_s=2N} M_E(p, q, \ell) \chi_\ell. \tag{35}$$

The  $M_E$  coefficients satisfy the ME with respect to the  $p, q$  indices. In addition,  $M_E(p_{\ell_1}, q_{\ell_1}, \ell_2) = \delta_{\ell_1, \ell_2}$ , where  $(p_{\ell_1}, q_{\ell_1})$  denotes the coordinates of the missing moments.

As explained in the previous examples, one can impose a normalization condition of the form  $\sum_{\ell=0}^{2N} \chi_\ell = 1$ , constraining  $\chi_0$ . Incorporating this within the above relation we have

$$u(p, q) = \hat{M}_E(p, q, 0) + \sum_{\ell=1}^{m_s=2N} \hat{M}_E(p, q, \ell) \chi_\ell \tag{36}$$

where

$$\hat{M}_E(p, q, \ell) = \begin{cases} M_E(p, q, 0) & \ell = 0 \\ M_E(p, q, \ell) - M_E(p, q, 0) & \ell \geq 1. \end{cases} \tag{37}$$

From the positivity theorems of the moment problem, we have to impose the moment constraints arising from the integral relations

$$\iint d\omega dv \Omega_\sigma(\omega, v) \left( \sum_{i,j \in [0, I]^2} \tilde{C}_{i,j} \omega^i v^j \right)^2 \psi(\omega, v) > 0 \tag{38}$$

for arbitrary  $\tilde{C}$ 's (not all zero), where

$$\Omega_\sigma(\omega, v) = \begin{cases} 1 & \sigma = 0 \\ \omega & \sigma = 1 \\ v & \sigma = 2 \\ a^2 - \omega - v & \sigma = 3. \end{cases} \tag{39}$$

It is implicitly assumed that  $\psi$  is zero outside the triangular domain of interest.

These integral inequalities become linear inequalities, with respect to the  $u$ -moments:

$$\sum_{i_1, j_1} \sum_{i_2, j_2} \tilde{C}_{i_1, j_1} \left( \sum_{n=1}^3 f_{\sigma, n} u(\lambda_{1; \sigma, n} + i_1 + i_2, \lambda_{2; \sigma, n} + j_1 + j_2) \right) \tilde{C}_{i_2, j_2} > 0 \tag{40}$$

where

$$f_{\sigma, n} = \begin{cases} 1, 0, 0 & \text{for } \sigma = 0 \\ 0, 1, 0 & \text{for } \sigma = 1 \\ 0, 0, 1 & \text{for } \sigma = 2 \\ a^2, -1, -1 & \text{for } \sigma = 3 \end{cases} \tag{41}$$

and the  $\lambda$ 's associated with nonzero  $f_{\sigma, n}$ 's

$$(\lambda_{1; \sigma, n}, \lambda_{2; \sigma, n}) = \begin{cases} (0, 0) & \text{for } \sigma = 0 \quad n = 1 \\ (1, 0) & \text{for } \sigma = 1 \quad n = 2 \\ (0, 1) & \text{for } \sigma = 2 \quad n = 3 \\ (0, 0), (1, 0), (0, 1) & \text{for } \sigma = 3. \end{cases} \tag{42}$$

**Table 1.** Ground state energy bounds ( $m = 0, I = 2$ ).

$\frac{b}{a}$	Bounds	$\frac{b}{a}$	Bounds
0.80	$6 < E < 30$	0.20	$292.6 < E < 295.5$
0.75	$26 < E < 33$	0.15	$496 < E < 506$
0.70	$33.8 < E < 35.2$	0.10	$1064 < E < 1093$
0.65	$38.8 < E < 39.4$	0.09	$1300 < E < 1340$
0.60	$44.33 < E < 44.42$	0.08	$1630 < E < 1680$
0.55	$50.98 < E < 51.03$	0.07	$2110 < E < 2180$
0.50	$59.54 < E < 59.58$	0.06	$2850 < E < 2950$
0.45	$70.85 < E < 70.92$	0.05	$4070 < E < 4210$
0.40	$86.32 < E < 86.44$	0.04	$6320 < E < 6520$
0.35	$108.30 < E < 108.70$	0.03	$11\ 160 < E < 11\ 520$
0.30	$141.60 < E < 142.20$	0.02	$24\ 950 < E < 25\ 800$
0.25	$195.60 < E < 196.80$	0.01	$99\ 170 < E < 102\ 970$

**Table 2.** Ground state energy bounds ( $m = 0, I = 3$ ).

$\frac{b}{a}$	Bounds	$\frac{b}{a}$	Bounds
0.40	$86.37 < E < 86.39$	0.10	$1077 < E < 1080$
0.30	$141.90 < E < 141.94$	0.05	$4120 < E < 4135$
0.20	$293.92 < E < 294.00$		

If one defines a coordinate pair sequence  $(i_l, j_l) \in [0, I] \times [0, I]$ , then the set of points covered by  $(i_{l_1}, j_{l_1}) + (i_{l_2}, j_{l_2}) + (\lambda_{1;\sigma,n}, \lambda_{2;\sigma,n})$ , lie within a square grid  $[0, N]^2$ , where  $N = 2I + 1$ . All the moments within this grid will be generated by the missing moments, previously defined.

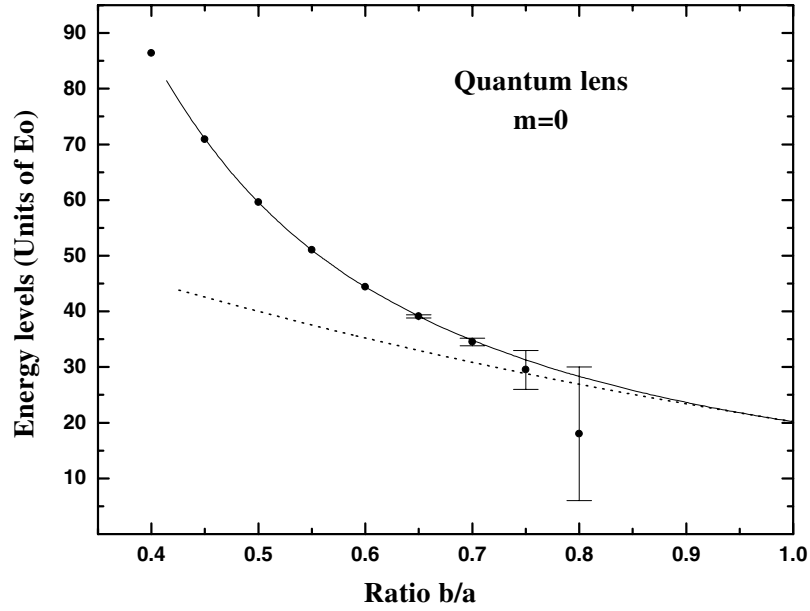
One proceeds by substituting the moment–missing moment relation in equation (34) into (40). This defines an infinite set of linear inequalities in the missing moments, and can be analyzed through the linear programming based EMM algorithm. The EMM numerical analysis generates a finite number of optimal  $\tilde{C}$ 's which determine if, to order  $I$ , the (normalized) inequalities in equation (40) have a solution set,  $\mathcal{U}_E^{(I)}$ , for the specified  $E$  value. The feasible energies define the converging lower and upper bounds.

In tables 1 and 2 we give some results of our approach, as a function of the ratio  $\frac{b}{a}$ , for the  $m = 0$  case. Note that  $a = 1$  in all the cases considered in this work. Already, for  $I = 2$  ( $m_s = 10$ ), and  $I = 3$  ( $m_s = 14$ ), we obtain very good bounds for the ground state energy, even for small lens thickness. As the ratio  $\frac{b}{a}$  becomes smaller, the lens becomes thinner, with maximum thickness  $b$ , and base diameter  $2a$ .

In figure 2, we compare the normalized ground state energy ( $\frac{E}{E_0}$ ), for  $m = 0$ , as a function of the ratio  $\frac{b}{a}$ , obtained by three methods:

- (i) exact numerical solution (solid curve) of equation (28);
- (ii) perturbation theory (dashed curves), based on a conformal transformation into a semi-spherical shape (Rodriguez *et al* 2001);
- (iii) EMM analysis, as reported in table 1 (solid black dots for the lower and upper bounds, when the ‘bounding’ bars become too small).

It can be seen that very good agreement is obtained between the exact solution and the EMM bounds, for  $\frac{b}{a} < 0.7$ . The perturbation results yield better agreement with the exact, numerical solution, for  $\frac{b}{a} > 0.8$ .



**Figure 2.** Ground state energy for a quantum lens as a function of the ratio  $\frac{b}{a}$ . The energy is given in units of  $E_0 = \frac{\hbar^2}{2ma^2}$ , as calculated by: exact numerical solution (solid curve); perturbation theory with respect to the  $\frac{b}{a}$  parameter (dashed curve, Rodriguez *et al* (2001)); and EMM theory, as given in table 1 (solid black dots). The lower and upper energy bounds are represented by ‘bounding’ bars (which cannot be depicted for smaller  $\frac{b}{a}$  values).

#### 4. The $m \neq 0$ moment equation

Within each symmetry class, the lowest lying state also corresponds to a non-negative configuration. Thus it is possible to extend the previous analysis to such states.

We first note that for the excited states, the wavefunction must be zero along the  $\rho = 0$  axis. This readily follows for the  $m = \text{odd}$  case, since  $\Psi(x, y, z) = e^{-im\phi}\psi(\rho, z)$ , and  $\Psi$  suffers a discontinuous behavior at the origin (i.e.  $\phi : 0 \rightarrow \pi$ ), with respect to variations in  $x$ , if  $m \neq 0$  and  $\psi(\rho = 0, z) \neq 0$ . To avoid such discontinuities,  $\psi(\rho = 0, z) = 0$ . More generally, one can argue that

$$\psi(\rho, z) = \rho^m \Omega_m(\rho, z) \quad (43)$$

where  $m \geq 0$ .

Let us now work, not with  $\Omega$ , but instead with

$$\phi(\rho, z) = \rho^m \psi(\rho, z). \quad (44)$$

Thus,  $\psi(\rho, z) = \rho^{-m}\phi(\rho, z)$ , and upon substituting in the differential equation for  $\psi$ :

$$-\frac{1}{\rho}\partial_\rho(\rho\partial_\rho\psi) + \frac{m^2}{\rho^2}\psi - \partial_z^2\psi = E\psi \quad (45)$$

we obtain

$$-\left(\frac{1}{\rho}\partial_\rho(\rho\partial_\rho\phi) + \partial_z^2\phi\right) + \frac{2m}{\rho}\partial_\rho\phi = E\phi. \quad (46)$$

Note that  $\phi(\rho = 0, z) = 0$ . This is an important factor in affirming the validity (i.e. uniqueness issues) of the ME resulting from equation (46).

**Table 3.** Lowest state energy bounds ( $m = 1$ ).

$\frac{b}{a}$	Bounds ( $I = 2$ )	Bounds ( $I = 3$ )
0.60	$64.1 < E < 64.4$	$64.222 < E < 64.230$
0.50	$82.50 < E < 82.67$	$82.596 < E < 82.599$
0.40	$113.78 < E < 114.26$	$114.050 < E < 114.056$
0.30	$176.15 < E < 177.97$	$177.15 < E < 177.20$
0.20	$339.6 < E < 348.6$	$344.0 < E < 344.4$
0.10	$1137.0 < E < 1208.5$	$1170.0 < E < 1175.0$

**Table 4.** Lowest state energy bounds ( $m = 2$ ).

$\frac{b}{a}$	Bounds ( $I = 2$ )	Bounds ( $I = 3$ )
0.60	$86.7 < E < 87.1$	$86.890 < E < 86.900$
0.50	$108.18 < E < 108.67$	$108.476 < E < 108.480$
0.40	$143.81 < E < 145.10$	$144.601 < E < 144.609$
0.30	$212.70 < E < 217.10$	$215.29 < E < 215.38$
0.20	$387.10 < E < 406.1$	$397.0 < E < 397.8$
0.10	$1206.0 < E < 1335.0$	$1263.0 < E < 1278.0$

Comparing equations (46) and (21), for the  $m = 0$ , case, we see that both are similar, except for the additional derivative term  $\frac{2m}{\rho} \partial_\rho \phi = -4m \partial_\omega \phi$ . In generating the corresponding ME, no boundary terms are introduced, and the only modification to equation (34) is the additional ‘ $-mp$ ’ term appearing in the coefficient of the  $u(p - 1, q)$  term:

$$\begin{aligned}
 -\frac{E}{4} u(p, q) &= R_2^2 p(p-1) u(p-2, q) - \left[ mp + p^2 + \frac{3p}{2} + 2pq \right] u(p-1, q) \\
 &\quad - 2R_1^2 pq u(p-1, q-1) + \left[ q^2 + \frac{q}{2} \right] u(p, q-1) \\
 &\quad + R_1^2 q(q-1) u(p, q-2)
 \end{aligned} \tag{47}$$

where  $p, q \geq 1$ , and

$$u(p, q) \equiv \iint_{\mathcal{D}} d\omega dv \omega^p v^q \phi(\omega, v) \tag{48}$$

where the domain of integration,  $\mathcal{D}$ , is the same as that in equation (31).

The results of this analysis are given in tables 3 and 4. They are in keeping with the nature of the previous results for the  $m = 0$  case.

## 5. Generalization to excited states

The ME in equation (47) is valid for any state. Within each  $m$  (azymuthal) quantum number symmetry class, the ‘excited’ states will have varying signature. However, if they are bounded, then one can generate converging bounds for their energy values, provided one can find a positive constant,  $c$ , such that

$$\phi_c(\omega, v) \equiv c + \phi(\omega, v) \geq 0 \tag{49}$$

for  $(\omega, v) \in \mathcal{D}$ , as defined previously. One can now replace equation (47) with the moments  $u(p, q) = u_c(p, q) - cv(p, q)$ , where  $u_c$  are the moments of the  $\phi_c$  configuration, and  $v(p, q) = \iint_{\mathcal{D}} d\omega dv \omega^p v^q$ . Thus, the new ME becomes an inhomogeneous relation. We can empirically determine appropriate  $c$  values by determining the existence of generated bounds for the energy. If a too large ‘ $c$ ’ value is used, then the generated bounds converge more slowly.

For the states discussed in sections 3 and 4, we know that  $c = 0$ .

This approach, referred to as the ‘C-Shift EMM’ approach, has been discussed in earlier works by Handy and Lee (1991). We do not discuss its implementation here.

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## Appendix

As indicated in the introduction, we provide here a pedagogic overview of EMM in the context of 1-space dimension problems. We do this for two reasons. The first is to make this work self-contained, thereby facilitating the reader’s understanding of EMM. The second is to contrast how an improper selection of  $\mathcal{P}_z$ , as discussed in the introduction, can prevent EMM from generating converging bounds to the ground state energy. In section A of this appendix, we review EMM. In section B, we focus on the proper selection of  $\mathcal{P}_z$ , within the real line,  $\text{Re}$ . In section C, we discuss the Hausdorff moment problem corresponding to the one-dimensional infinite well potential. This serves to complete the discussion with respect to one-dimensional compact domains, facilitating the understanding of the infinite quantum lens problem, and the removal of the boundary term relations from the pertinent ME.

### Appendix A. The sextic anharmonic oscillator

#### A. 1. Hamburger moment formulation

Consider the sextic anharmonic oscillator potential problem:

$$-\epsilon \partial_x^2 \Psi(x) + (mx^2 + gx^6)\Psi(x) = E\Psi(x) \quad (\text{A.1})$$

where the kinetic energy perturbation parameter,  $\epsilon$ , is explicitly noted, for later reference. The mass and coupling strength parameters are denoted by  $m$  and  $g$ , respectively.

The signature structure for the ground ( $\Psi_0$ ) and first excited ( $\Psi_1$ ) states are known *a priori*:  $\Psi_i(x) = x^i \Upsilon_i(x)$ , where  $\Upsilon_i(x) > 0$ . For simplicity, we confine our analysis to the ground state case.

Define the Hamburger power moments

$$\mu(p) = \int_{-\infty}^{+\infty} dx x^p \Psi(x) \quad (\text{A.2})$$

$p \geq 0$ . Upon multiplying both sides of the Schrödinger equation by  $x^p$ , and performing the necessary integration by parts, we obtain the ME

$$g\mu(p+6) = -m\mu(p+2) + E\mu(p) + \epsilon p(p-1)\mu(p-2) \quad (\text{A.3})$$

for  $p \geq 0$ . This corresponds to an effective sixth order finite difference equation, in which specification of the ‘initialization’ moments, or *missing moments*,  $\{\mu(\ell) | 0 \leq \ell \leq 5\}$ , as well as the energy parameter,  $E$ , generates all of the remaining moments.

One important aspect about working within a moments’ representation is that kinetic energy expansions become regular (i.e.  $\epsilon$  expansions). This is not the case in configuration space, requiring the use of singular perturbation type methods (Bender and Orszag 1978). One immediate impact of the regularity in  $\epsilon$  is that the order of the ME does not change for  $\epsilon = 0$  and  $0^+$  (unlike in configuration space, where the order of the differential equation abruptly changes from zero to two).

Let us denote the missing moment order by  $1 + m_s$ , where  $m_s = 5$ . We can express the linear dependence of the moments on the missing moments through the expression

$$\mu(p) = \sum_{\ell=0}^{m_s} M_E(p, \ell) \mu(\ell) \quad (\text{A.4})$$

where

$$M_E(\ell_1, \ell_2) = \delta_{\ell_1, \ell_2} \quad (\text{A.5})$$

for  $0 \leq \ell_1, \ell_2 \leq m_s$ . The  $M_E$  coefficients are readily obtainable, since they satisfy the ME relation with respect to the  $p$ -index, in addition to the preceding initialization conditions.

We must also impose some, convenient, normalization condition. This can be chosen to be

$$\sum_{\ell=0}^{m_s} \mu(\ell) = 1. \quad (\text{A.6})$$

Constraining the zeroth order moment,  $\mu(0) = 1 - \sum_{\ell=1}^{m_s} \mu(\ell)$ , we redefine the moment-missing moment relation as

$$\mu(p) = \sum_{\ell=0}^{m_s} \hat{M}_E(p, \ell) \hat{\mu}(\ell) \quad (\text{A.7})$$

where

$$\hat{\mu}(\ell) = \begin{cases} 1 & \text{for } \ell = 0 \\ \mu(\ell) & \text{for } 1 \leq \ell \leq m_s \end{cases} \quad (\text{A.8})$$

and

$$\hat{M}_E(p, \ell) = \begin{cases} M_E(p, 0) & \text{for } \ell = 0 \\ M_E(p, \ell) - M_E(p, 0) & \text{for } 1 \leq \ell \leq m_s. \end{cases} \quad (\text{A.9})$$

From the moment problem, we know that the moments of a non-negative measure, on the entire real axis, must satisfy the HH constraints

$$\int_{-\infty}^{+\infty} dx \left( \sum_{i=0}^I C_i x^i \right)^2 \Psi(x) \geq 0 \quad (\text{A.10})$$

for arbitrary  $C_i$ 's (not all zero), and  $0 \leq I < \infty$ . The zero equality is only possible for configurations made up of a finite number of Dirac distributions.

The HH integral constraints can be transformed into the quadratic form expression

$$\sum_{i_1, i_2=0}^I C_{i_1} \mu(i_1 + i_2) C_{i_2} > 0. \quad (\text{A.11})$$

These inequalities do not guarantee uniqueness for  $\Psi$  (i.e. that the physical solution is the only one with these moments); however, because we are implicitly working with the moments of a physical system, for which there is uniqueness, the nature of the  $\hat{M}_E(p, \ell)$  matrix coefficients should guarantee uniqueness as well, within the moments' representation, i.e. satisfaction of the Carlemann conditions, etc (for further details see Bender and Orszag 1978).

One can then substitute the moment-missing moment relation

$$\sum_{\ell=0}^{m_s} \left( \sum_{i_1, i_2=0}^I C_{i_1} \hat{M}_E(i_1 + i_2, \ell) C_{i_2} \right) \hat{\mu}(\ell) > 0 \quad (\text{A.12})$$

which generates an uncountable number of linear inequalities (i.e. one linear inequality for each  $C$ -tuple) in the (unconstrained) missing moment variable space:

$$\sum_{\ell=1}^{m_s} \mathcal{A}_\ell[C] \mu(\ell) < \mathcal{B}[C] \quad (\text{A.13})$$

where

$$\mathcal{A}_\ell[C] \equiv - \sum_{i_1, i_2=0}^I C_{i_1} \hat{M}_E(i_1 + i_2, \ell) C_{i_2} \quad (\text{A.14})$$

and

$$\mathcal{B}[C] \equiv \sum_{i_1, i_2=0}^I C_{i_1} \hat{M}_E(i_1 + i_2, 0) C_{i_2}. \quad (\text{A.15})$$

We recall that the missing moments are restricted to  $\sum_{\ell=0}^{m_s} \mu(\ell) = 1$ .

Let  $\mathcal{U}_E^{(I)}$  denote the (convex) solution set to the above set of HH inequalities, for given  $E$  and  $I$ . The objective is to determine the feasible energy interval, to order  $I$ , for which convex solution sets exists:

$$E \in (E_L^{(I)}, E_+^{(I)}) \quad \text{if} \quad \mathcal{U}_E^{(I)} \neq \emptyset. \quad (\text{A.16})$$

This can be done through a linear programming based *cutting method* that finds the optimal  $C$ 's leading to a quick assessment on the existence or nonexistence of  $\mathcal{U}_E^{(I)}$  (Handy *et al* (1988a, b)).

The preceding formalism is appropriate if the Schrödinger equation potential is not symmetric. In the present case, since the potential is symmetric, we can define a more efficient representation by working in terms of a Stieltjes moment formulation. This is done in the following section.

### A. 2. Stieltjes moment formulation

The parity invariant nature of the sextic anharmonic oscillator requires that the ground state be symmetric,  $\Psi(-x) = \Psi(x)$ . This in turn introduces more moment constraints.

For symmetric configurations, the odd order Hamburger moments are zero,  $\mu(\text{odd}) = 0$ . The even order Hamburger moments can be regarded as the moments of a Stieltjes measure restricted to the non-negative real axis (through a change of variables,  $y = x^2$ )

$$u(\rho) \equiv \mu(2\rho) \quad (\text{A.17})$$

where

$$u(\rho) = \int_0^\infty dy y^\rho \Phi(y) \quad (\text{A.18})$$

and

$$\Phi(y) = \frac{\Psi(\sqrt{y})}{\sqrt{y}}. \quad (\text{A.19})$$

The Stieltjes moments also satisfy a ME ( $\epsilon = 1$ ):

$$gu(\rho + 3) = -mu(\rho + 1) + Eu(\rho) + 2\rho(2\rho - 1)u(\rho - 1) \quad (\text{A.20})$$

$\rho \geq 0$ .

The order of this finite difference ME is  $1 + m_s = 3$ , leading to the representation

$$u(\rho) = \sum_{\ell=0}^{m_s} \hat{\mathcal{M}}_E(\rho, \ell) \hat{u}(\ell) \quad (\text{A.21})$$

where the  $\hat{u}(\ell)$  are defined as before, and satisfy the constraint,  $\sum_{\ell=0}^{m_s} u(\ell) = 1$ .



One important aspect of working with Stieltjes moments is that because the underlying function must be positive, all the Stieltjes moments must also be positive (which is not the case for the Hamburger moments). Thus, for the adopted normalization condition, we have

$$0 < u(\ell) < 1 \quad (\text{A.22})$$

for  $0 \leq \ell \leq m_s (=2)$ .

Since one is working on the non-negative real axis,  $y \geq 0$ , more HH constraints are possible. The constraints in equation (A.11), arising from the integral expression in equation (A.10), define the necessary and sufficient conditions for the moments to correspond to a non-negative measure on the entire real axis. If we pretend that  $\Phi(y)$  exists on the entire real axis, but we want it to be zero on the negative real axis, then one must also introduce the counterpart to equation (A.10) for the configuration  $y\Phi(y)$ :

$$\int dy y^\sigma \left( \sum_{i=0}^I C_i y^i \right)^2 \Phi(y) > 0 \quad (\text{A.23})$$

for  $\sigma = 0, 1$ , and  $I < \infty$ . Thus, the only way both  $\Phi(y)$  and  $y\Phi(y)$  can be non-negative on the entire  $y$ -axis is for  $\Phi(y) = 0$ , for  $y < 0$ . This is an intuitive way of motivating the HH–Stieltjes moment conditions for a non-negative measure defined on the non-negative real axis. Consequently, in terms of a quadratic form expression, we have

$$\sum_{i_1, i_2=0}^I C_{i_1} u(\sigma + i_1 + i_2) C_{i_2} > 0 \quad (\text{A.24})$$

for  $\sigma = 0, 1$  and  $I \geq 0$ .

Repeating the same analysis presented earlier (i.e. substituting the moment–missing moment relations, and implementing the linear programming based cutting procedure) allows us to generate very tight bounds for the ground state energy. In particular, for  $\epsilon = m = g = 1$ , one obtains

$$1.435\,624\,619\,0092 < E < 1.435\,624\,619\,0178 \quad (\text{A.25})$$

for  $I = 15$ .

## Appendix B. Defining quantizable EMM-moment equations

We now focus on issues of relevance to the application of EMM to the quantum lens problem. Consider the configuration  $F(x) = x^2\Psi(x)$ . Its Stieltjes moments (for symmetric solutions) will satisfy the ME derived from equation (A.20):

$$gw(\rho + 2) = -mw(\rho) + Ew(\rho - 1) + 2\rho(2\rho - 1)w(\rho - 2) \quad (\text{B.1})$$

$\rho \geq 2$ , where  $w(\rho) \equiv u(\rho + 1)$ . This corresponds to an effective  $1 + m_s = 4$  order relation since the missing moments  $\{w(0), w(1), w(2), w(3)\}$  must be specified before all the other moments can be generated.

However, application of EMM, to the above ME, will not generate any discrete state energy bounds. The principal reason for this is that the same ME ensues if we multiply both sides of (the modified Schrödinger equation)

$$\left( -\partial_x^2 + mx^2 + gx^6 - E \right) \Psi(x) = \mathcal{D}(x) \quad (\text{B.2})$$

by  $x^{p+4}$ ,  $p \geq 0$ , provided  $\mathcal{D}(x)$  is a (symmetric) distribution which is projected out when multiplied by  $x^4$ . Thus, we can have  $\mathcal{D}(x) = A\delta(x) + B\delta''(x)$ , where  $A$  and  $B$  are arbitrary. It is reasonable to expect that equation (B.2) admits many bounded, positive, solutions, for arbitrary  $E$ ; thereby explaining the lack of any EMM generated bounds for the  $w$  moments.

In general, when generating a ME, we are free to multiply both sides of the the Schrödinger equation by expressions of the form  $x^p T(x)$  (where  $p \geq 0$ ) so long as all the zeros of  $T$  are zeros of the desired physical solution (i.e. if  $T(x_z) = 0$ , then  $\Psi(x_z) = 0$ ). If this is not satisfied, then the resulting ME relation will fail to distinguish between the true Schrödinger equation, and that modified by additional distribution terms supported at zeros of  $T$ .

In accordance with the above, whereas  $T(x) = x^4$  generates a ME that yields no discrete states, the function  $T(x) = 1+x^2$  does generate the ground state solution. Applying  $x^{2\rho}(1+x^2)$  to both sides of equation (A.1), we obtain the Stieltjes ME

$$gu(\rho + 4) = -gu(\rho + 3) - mu(\rho + 2) + (E - m)u(\rho + 1) \\ + [E + 2(\rho + 1)(2\rho + 1)]u(\rho) + 2\rho(2\rho - 1)u(\rho - 1). \quad (\text{B.3})$$

This is a  $1 + m_s = 4$  order relation. Application of EMM generates the ground state energy (although at a slower convergence rate):  $1.435\,6178 < E_{gr} < 1.435\,6185$ , utilizing Stieltjes moments  $\{u(\leq 30)\}$ .

A more instructive example is that of the first excited state for the sextic anharmonic oscillator. The wavefunction will be of the form  $\Psi_{exc}(x) = x\Upsilon_1(x)$ , where  $\Upsilon_1(x) > 0$ , and  $\Upsilon_1(-x) = \Upsilon_1(x)$ , for  $x \in \text{Re}_x$ . We can transform the Schrödinger equation into an equation for  $\Upsilon_1(x)$ :

$$-\epsilon \left( \frac{2}{x} \Upsilon_1'(x) + \Upsilon_1''(x) \right) + [mx^2 + gx^6]\Upsilon_1(x) = E\Upsilon_1(x). \quad (\text{B.4})$$

Integrating both sides with respect to  $x^{2\rho}$  will yield the corresponding Stieltjes ME; however, it will involve (for  $\rho = 0$ ) the non- $(\Upsilon_1)$  moment expression  $\int_{-\infty}^{+\infty} dx \frac{\Upsilon_1'(x)}{x}$ , which is finite. Although a corresponding EMM analysis can be implemented, it will require a modification of the conventional EMM formalism, as previously defined.

An alternate approach is to simply take  $T(x) \equiv x$ , and work with the configuration  $\Xi(x) \equiv x\Psi(x) = x^2\Upsilon_1(x)$ . The Stieltjes- $\Xi$  moments are  $w(\rho) \equiv \int_{-\infty}^{+\infty} dx x^{2\rho} \Xi(x)$ , for  $\rho \geq 0$ . In terms of the Hamburger moments, these become  $w(\rho) = \mu(2\rho + 1)$ . If we return to the Hamburger ME relation in equation (A.3), and take  $p = 2\rho + 1$ , we obtain the desired  $w$ -Stieltjes equation:

$$-\epsilon 2\rho(2\rho + 1)w(\rho - 1) + mw(\rho + 1) + gw(\rho + 3) = Ew(\rho) \quad (\text{B.5})$$

$\rho \geq 0$ . For the case  $\epsilon = m = g = 1$ , working with the first 30 Stieltjes moments, we obtain the bound

$$5.033\,395\,937\,697 < E_1 < 5.033\,395\,937\,709. \quad (\text{B.6})$$

For the ground state wavefunction, the function  $T(x)$  cannot be zero except where  $\Psi_{gr}(x)$  is zero. For problems defined on a compact domain, this means that  $T$  can be zero only at the boundary, where the ground state wavefunction will, generally, be zero. We discuss this in the following section.

### Appendix C. A Hausdorff moment problem: the infinite square well

We now consider the infinite square well problem

$$-\partial_x^2 \Psi(x) = E\Psi(x) \quad (\text{C.1})$$

where  $\Psi(\pm L) = 0$ . The Hamburger moments are  $\mu(p) = \int_{-L}^{+L} dx x^p \Psi(x)$ . For symmetric configurations, we have  $\mu(2\rho) \equiv u(\rho) = \int_0^{L^2} dy y^\rho \Phi(y)$ , where  $y \equiv x^2$  and  $\Phi(y) \equiv \frac{\Psi(\sqrt{y})}{\sqrt{y}}$ . In terms of these *Hausdorff* moments, the corresponding ME becomes

$$-2\rho(2\rho - 1)u(\rho - 1) - 2L^{2\rho} \Psi'(L) = E u(\rho) \quad (\text{C.2})$$

$\rho \geq 0$ . It involves the boundary terms at  $\pm L$ .

Relative to the Stieltjes problem, the Hausdorff moment problem introduces more constraints to the previous Stieltjes (HH) inequalities. We can, intuitively, derive these by assuming that  $\Phi(y)$  is non-negative on  $[0, \infty)$ . This is what the Stieltjes (HH) constraints in equation (A.23) guarantee (i.e. if we pretend that the Hausdorff moments are actually Stieltjes moments).

In order to further constrain such a function so that it is zero on the interval  $[L^2, \infty)$ , we must require that  $(L^2 - y)\Phi(y)$  be non-negative on  $[0, \infty)$ :

$$\int dy (L^2 - y) \left( \sum_{i=0}^I C_i y^i \right)^2 \Phi(y) > 0 \quad (\text{C.3})$$

$I < \infty$ . That is:

$$\sum_{i_1, i_2=0}^I C_{i_1} (L^2 u(i_1 + i_2) - u(1 + i_1 + i_2)) C_{i_2} > 0. \quad (\text{C.4})$$

This is the third set of HH constraints that must be added to those in equation (A.23), for the Hausdorff problem.

We can summarize all the Hausdorff–HH relations by

$$\sum_{i_1, i_2=0}^I C_{i_1}^{(\sigma)} (\Gamma_{\sigma}^{(1)} u(i_1 + i_2) + \Gamma_{\sigma}^{(2)} u(1 + i_1 + i_2)) C_{i_2}^{(\sigma)} > 0 \quad (\text{C.5})$$

for  $\sigma = 0, 1, 2$ , where

$$\Gamma_{\sigma}^{(1)} = \begin{cases} 1 & \sigma = 0 \\ 0 & \sigma = 1 \\ L^2 & \sigma = 2 \end{cases} \quad (\text{C.6})$$

and

$$\Gamma_{\sigma}^{(2)} = \begin{cases} 0 & \sigma = 0 \\ 1 & \sigma = 1 \\ -1 & \sigma = 2 \end{cases} \quad (\text{C.7})$$

for all nontrivial  $C^{(\sigma)}$ 's, and  $I \geq 0$ .

We outline how the above constraints lead to the quantization of the ground state.

Let  $L = 1$ , and  $A \equiv 2\Psi'(L)$ . Then  $u(0) = -\frac{A}{E} > 0$ , and all the remaining moments can be generated, once  $A$  is normalized. The first three Hausdorff–HH conditions ( $I = 0$ ) become:

$$\text{Hausdorff–HH relations } (I = 0) \rightarrow \begin{cases} u(0) > 0 \\ u(1) > 0 \\ u(0) - u(1) > 0. \end{cases} \quad (\text{C.8})$$

Combining  $Eu(1) = -2u(0) - A$ , and  $u(1) > 0$ , yields  $-2\frac{u(0)}{E} + u(0) > 0$ , or  $\frac{2}{E} < 1$ . The third inequality,  $\frac{u(1)}{u(0)} < 1$ , yields  $-\frac{2}{E} + 1 < 1$ , or  $E > 0$ ; hence the lower bound

$$2 < E. \quad (\text{C.9})$$

Having established the positivity of  $E$ , we are free to impose the normalization  $A = -1$ , hence  $u(0) = \frac{1}{E}$ . Thus, the ME relation effectively becomes a zero missing moment problem, with  $m_s = 0$ . We can proceed with a numerical determination of the ground state energy.

For problems corresponding to  $m_s = 0$ , we do not have to implement the linear programming based, EMM, formulation. Instead, we can work with the nonlinear HH

inequalities (which are the relations usually cited in the literature) corresponding to the quadratic form relations given previously. That is, the Hausdorff–HH linear (in the moments) constraints, are equivalent to the nonlinear (in the moments) determinantal relations:

$$\text{Det}(\Delta_{\sigma}^{(I)}) > 0 \quad (\text{C.10})$$

where the various HH matrices are

$$\Delta_{\sigma; i_1, i_2}^{(I)} = \Gamma_{\sigma}^{(1)} u(i_1 + i_2) + \Gamma_{\sigma}^{(2)} u(1 + i_1 + i_2) \quad (\text{C.11})$$

for  $\sigma = 0, 1, 2$ , and  $0 \leq i_1, i_2 \leq I$ .

The numerical evaluation of these inequalities yields the bounds

$$2.467\,401\,0541 < E < 2.467\,401\,1008 \quad (\text{C.12})$$

utilizing all the HH determinants corresponding to the first seven moments:  $\{u(\leq 6)\}$ . This compares exceptionally well (up to seven decimal places) with the true answer,  $E = (\frac{\pi}{2})^2$ .

### C.1. Moment equations with no boundary terms

In practice, particularly for multi-dimensional applications, we prefer to work with MEs that do not involve any boundary terms. For the infinite square well case, we can do so by multiplying both sides of the corresponding Schrödinger equation by  $x^p T(x)$ , where  $T(\pm 1) = 0$ . The ensuing ME will not involve any boundary terms because the kinetic energy term becomes

$$\int_{-1}^{+1} dx G(x) \Psi''(x) = G \Psi' \Big|_{-1}^{+1} - G' \Psi \Big|_{-1}^{+1} + \int_{-1}^{+1} dx G''(x) \Psi(x) \quad (\text{C.13})$$

where  $G(x) \equiv x^p T(x)$ . Since both  $G$  and  $\Psi$  are zero at the boundary, no boundary terms will contribute to the ensuing ME relation.

As an example, let  $T(x) = 1 - x^2$ , for the  $L = 1$  case. Applying  $x^{2\rho}(1 - x^2)$  to both sides of the infinite square well problem yields the Hausdorff ME

$$Eu(\rho + 1) = [E - (2\rho + 2)(2\rho + 1)]u(\rho) + 2\rho(2\rho - 1)u(\rho - 1) \quad (\text{C.14})$$

for  $\rho \geq 0$ . Application of EMM duplicates the bounds previously cited.

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