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New identities from quantum-mechanical sum rules of parity-related potentials

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Abstract

We apply quantum-mechanical sum rules to pairs of one-dimensional systems defined by potential energy functions related by parity. Specifically, we consider symmetric potentials, $V(x) = V(-x)$, and their *parity-restricted* partners, ones with $V(x)$ but defined only on the positive half-line. We extend recent discussions of sum rules for the quantum bouncer by considering the *parity-extended* version of this problem, defined by the symmetric linear potential, $V(z) = F|z|$ and find new classes of constraints on the zeros of the Airy function, $Ai(\zeta)$, and its derivative, $Ai'(\zeta)$. We also consider the parity-restricted version of the harmonic oscillator and find completely new classes of mathematical relations, unrelated to those of the ordinary oscillator problem. These two soluble quantum-mechanical systems defined by power-law potentials provide examples of how the form of the potential (both parity and continuity properties) affects the convergence of quantum-mechanical sum rules. We also discuss semi-classical predictions for expectation values and the Stark effect for these systems.

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1. Introduction

Sum rules, constraints on energy-difference weighted combinations of on- and off-diagonal matrix elements, have been an important theoretical construct in quantum mechanics since its earliest days. For example, the Thomas–Reiche–Kuhn (TRK) [1] sum rule was one of the earliest quantitative checks on the oscillator strengths of atomic transitions and an important confirmation of the applicability of quantum mechanics to atomic systems. Their use continues today, for example, with QCD sum rules used to probe the masses of both light and heavy quarks in hadronic systems. For a list of recent applications of sum rules, see [2].

The study of sum rules and how such constraints are realized [2] can provide useful examples of a variety of mathematical techniques utilized for their confirmation. In addition, sum rules can be used to generate new mathematical constraints [3] on quantities involving infinite sums. For example, in exactly that context, two of us have recently shown how it is possible to systematically derive new constraints on the zeros, $(-\zeta_n)$, of the Airy function, $Ai(\zeta)$, of the form $S_p(n) = \sum_{k \neq n} (\zeta_k - \zeta_n)^{-p}$ for the natural values of $p \geq 2$ using quantum-mechanical sum rules applied to the so-called quantum bouncer problem [4]. Defined by the potential

$$V(z) = \begin{cases} Fz & \text{for } z > 0 \\ \infty & \text{for } z < 0, \end{cases} \quad (1)$$

this quantum-mechanical problem has been applied to recent novel experiments, ranging from the bound states of neutrons in the Earth's gravitational field [5] to optical analogs of gravitational wave packets [6] which demonstrate the presence of predicted [7] wave packet revivals.

In our earlier study, a number of the most well-known sum rules did not converge due to the lack of continuity of the bouncer potential at the origin. In this note, we extend the results of [4] to discuss mathematical constraints which arise from the study of quantum-mechanical sum rules in a closely related system, namely the symmetric linear potential, defined by

$$V(z) = F|z|. \quad (2)$$

This is an example of a *parity-extended* potential, namely taking the one that is defined only for $z > 0$, and extending it in a symmetric way over the real axis. In this case, we find new relationships involving *both* the zeros of $Ai(\zeta)$ *and* its derivative $Ai'(\zeta)$, namely $-\zeta_n$ and $-\eta_n$, respectively. In section 3 we also explore the convergence properties of sum rules in this system, compared to the quantum bouncer, because of the improved mathematical behavior of the potential energy function in this case.

For comparison, we also consider in section 5 a *parity-restricted* version of the most well-studied system in quantum mechanics, namely the harmonic oscillator. Specifically, we examine the structure of sum rules in the 'half'-SHO potential, defined by

$$V(x) = \begin{cases} m\omega^2 x^2/2 & \text{for } x \geq 0 \\ \infty & \text{for } x < 0 \end{cases} \quad (3)$$

and find dramatically different behavior for many sum rules.

We are motivated to study the relation between such parity-related potentials since the solution space of the parity-restricted version of a symmetric potential, $V(x) = V(-x)$, consists solely of the odd energy eigenvalues and eigenstates, with only a trivial change in normalization. Thus, half of the wavefunctions and energies will be closely related in the two systems. Since sum rules involve intricate relationships between energy differences and matrix elements derived from the wavefunctions, it is instructive to see how identical sum rules are realized in two parity-related systems. We find that many matrix elements can be very different in character between two such related systems, yielding sum rule identities which are realized in novel ways.

For these two systems, we then make contact with semi-classical (WKB-like) probability distributions (in section 6) and examine the similarities with the new exact quantum results presented here in the large n limit. We also note that a recent examination of the Stark effect in the symmetric linear potential [8] has found interesting constraints on second-order perturbation theory (PT) sums which are very similar to the energy-weighted sum rules we will discuss below, and we extend that analysis to the 'half'-SHO system introduced here, allowing for insight into the structure of the Stark effect in that system. We begin by briefly reviewing the results of [8] in the next section, mostly to establish notation.

2. Solutions for the symmetric linear potential

We begin by reviewing the properties of the solutions for the symmetric linear potential in equation (2), using a slight modification of the notation in [8]. We note that the only difference in notation with [4] is in the normalization of the wavefunctions, corresponding only to a physically irrelevant difference in phase.

Using the fact that the linear potential admits Airy function solutions, with different forms for positive and negative values of position, we can construct piecewise-continuous solutions of the corresponding Schrödinger equation. Because of the symmetry properties of the potential, we can also classify the solutions by their parity, with the odd functions, which must vanish at the origin, related to the solutions of the quantum bouncer problem. For background on the solutions to the bouncer problem, see also [7, 9, 10].

Specifically, the odd solutions can be written in the form

$$\psi_n^{(-)}(z) = N_n^{(-)} \begin{cases} Ai(z/\rho - \beta_n) & \text{for } 0 \leq z \\ -Ai(-z/\rho - \beta_n) & \text{for } z \leq 0, \end{cases} \quad (4)$$

where $\rho \equiv (\hbar^2/2mF)^{1/3}$. The appropriate boundary condition at the origin is that the wavefunction must vanish there which implies that

$$\psi_n^{(-)}(0) = Ai(-\beta_n), \quad (5)$$

where we identify $\beta_n = \zeta_n$ where the $-\zeta_n$ are the zeros of $Ai(\zeta)$. The corresponding combination for even parity solutions is written as

$$\psi_n^{(+)}(z) = N_n^{(+)} \begin{cases} Ai(z/\rho - \beta_n) & \text{for } 0 \leq z \\ Ai(-z/\rho - \beta_n) & \text{for } z \leq 0, \end{cases} \quad (6)$$

which at the origin must satisfy $[\psi_n^{(+)}(z=0)]' = 0$, implying that $\beta_n = \eta_n$ where the $-\eta_n$ are the zeros of $Ai'(\zeta)$.

Handbook results [11, 12] give approximations for these zeros, in the large n limit, as

$$\zeta_n \sim \left[\frac{3\pi}{4}(2n - 1/2) \right]^{2/3} \quad \text{and} \quad \eta_n \sim \left[\frac{3\pi}{4}((2n - 1) - 1/2) \right]^{2/3}, \quad (7)$$

where the labeling starts with $n = 1$ in both cases. We note that WKB quantization gives the same results [8], valid for large quantum numbers.

The normalizations required in equations (4) and (6) are obtained by using integrals first derived by Gordon [13] and Albright [14] collected in appendix A, specifically equation (A.7), and are given by

$$N_n^{(-)} = \frac{1}{\sqrt{2\rho}Ai'(-\zeta_n)} \quad \text{and} \quad N_n^{(+)} = \frac{1}{\sqrt{2\rho\eta_n}Ai(-\eta_n)}. \quad (8)$$

We note that the wavefunctions at the origin satisfy

$$\psi_n^{(-)}(0) = 0 \quad \text{and} \quad \psi_n^{(+)}(0) = \frac{1}{\sqrt{2\rho\eta_n}}. \quad (9)$$

The energy eigenvalues are then given directly in terms of the ζ_n, η_n by

$$E_n^{(-)} = \mathcal{E}_0\zeta_n \quad \text{and} \quad E_n^{(+)} = \mathcal{E}_0\eta_n, \quad (10)$$

where $\mathcal{E}_0 \equiv \rho F$ and the energy spectrum satisfies

$$E_1^{(+)} < E_1^{(-)} < E_2^{(+)} < E_2^{(-)} < \dots \quad (11)$$

Just as for the bouncer system [10], we have a power-law potential of the form $V_{(k)}(x) = V_0|x/a|^k$, and the quantum-mechanical virial theorem, $\langle \hat{T} \rangle = \frac{k}{2}\langle \hat{V} \rangle$, is satisfied for

$k = 1$ which we can confirm by direct evaluation. For example, for odd states we have the matrix elements

$$\begin{aligned} \langle \psi_n^{(-)} | V(z) | \psi_n^{(-)} \rangle &= \int_{-\infty}^{+\infty} |\psi_n^{(-)}(z)|^2 F|z| dz \\ &= \frac{2F\rho^2}{2\rho[Ai'(-\zeta_n)]^2} \int_0^\infty y[Ai(y - \zeta_n)]^2 dy \\ &= \frac{2}{3}\mathcal{E}_0\zeta_n = \frac{2}{3}E_n^{(-)}, \end{aligned} \tag{12}$$

using the integral in equation (A.8), with a similar result for the expectation value of the potential energy for the even states. The expectation value of the kinetic energy operator,

$$\langle \psi_n^{(\pm)} | \hat{T} | \psi_n^{(\pm)} \rangle = \frac{1}{2m} \langle \psi_n^{(\pm)} | \hat{p}^2 | \psi_n^{(\pm)} \rangle = \frac{1}{3}E_n^{(\pm)}, \tag{13}$$

can be evaluated by either (i) using the definition of the Airy differential equation, $Ai''(\zeta - \beta) = (\zeta - \beta)Ai(\zeta)$, to rewrite the integral in terms of the one in equation (A.8) or (ii) using an integration by parts to move one derivative onto the first wavefunction, and then using the integral in equation (A.10).

The dipole matrix elements needed for many of the best-known sum rules have a different form than in the quantum bouncer. Using the symmetry of the potential, we have

$$\langle \psi_n^{(-)} | z | \psi_n^{(-)} \rangle = \langle \psi_n^{(+)} | z | \psi_n^{(+)} \rangle = 0, \tag{14}$$

while using equation (A.12), we find that

$$\langle \psi_n^{(-)} | z | \psi_k^{(+)} \rangle = \frac{-2\rho}{\sqrt{\eta_k}(\eta_k - \zeta_n)^3}. \tag{15}$$

As with all of the matrix element expressions and sum rule identities we present, we have confirmed these expressions numerically using *Mathematica*[®].

In contrast to the quantum bouncer problem [4] where all off-diagonal matrix elements gave terms proportional to the inverse powers of $(\zeta_n - \zeta_k)$, using sum rules involving only dipole-matrix elements for the symmetric linear potential will give constraints on sums of powers of $1/(\eta_k - \zeta_n)$. Matrix elements for even powers of z , for example

$$\langle \psi_n^{(\pm)} | z^2 | \psi_n^{(\pm)} \rangle, \tag{16}$$

will connect even–even and odd–odd states. The corresponding odd–odd sum rules will reproduce some of the same identities found in [4], while the even–even sum rules will generate new identities, involving sums over inverse powers of $(\eta_k - \eta_n)$.

3. New constraints from the symmetric linear potential

To illustrate the range of new constraints which the symmetric linear potential places on the ζ_n and η_n , we first consider the most well-known sum rules involving dipole matrix elements. The famous TRK sum rule [1] is given by

$$\sum_{k \neq n} (E_k - E_n) |\langle n | z | k \rangle|^2 = \frac{\hbar^2}{2m}, \tag{17}$$

while a completeness relation for the matrix elements of the momentum operator can be written in terms of dipole matrix elements as

$$\sum_{k \neq n} (E_k - E_n)^2 |\langle n | z | k \rangle|^2 = \frac{\hbar^2}{m^2} \langle n | \hat{p}^2 | n \rangle = \frac{2\hbar^2}{m} [E_n - \langle n | V(z) | n \rangle]. \tag{18}$$

We note that since the states n and k that contribute to the sum rule will be of opposite parity, the $k \neq n$ restriction is unnecessary and we can sum over all intermediate state k labels.

Two other sum rules involving dipole matrix elements have been discussed by Bethe and Jackiw [15, 16], namely

$$\sum_k (E_k - E_n)^3 |\langle n|z|k \rangle|^2 = \frac{\hbar^4}{2m^2} \left\langle n \left| \frac{d^2V(z)}{dz^2} \right| n \right\rangle \tag{19}$$

and

$$\sum_k (E_k - E_n)^4 |\langle n|z|k \rangle|^2 = \frac{\hbar^4}{m^2} \left\langle n \left| \left(\frac{dV(z)}{dz} \right)^2 \right| n \right\rangle, \tag{20}$$

which are sometimes called the *force times momentum* and *force-squared* sum rules, respectively. We note that not all such sum rules necessarily lead to convergent expressions. In [4], equations (19) and (20) could not be applied in the quantum bouncer system due to the discontinuous nature of the potential in equation (1). In the case of the symmetric linear potential, the system is defined by a continuous potential and even the discontinuous derivative will lead to a convergent result in the corresponding sum rule in equation (19). These results regarding convergence are consistent with the form of the dipole matrix elements in equation (15), where their values for fixed k or n clearly decrease more quickly with increasing n or k than their counterparts in the bouncer system, indicating better convergence.

When we fix the state labeled n as being one of the odd solutions and sum over k values corresponding to the even states, the $1/\sqrt{\eta_k}$ factors remain inside the summation, giving sums of the form

$$T_p(n) \equiv \sum_{\text{all } k} \frac{1}{\eta_k (\eta_k - \zeta_n)^p}. \tag{21}$$

In contrast, when the even states are fixed, switching the roles of n and k in equation (15), then the common $1/\sqrt{\eta_n}$ factor can be removed from inside the summation and eventually moved to the right-hand side of the identity involved. In those cases, we find expressions of the form

$$U_p(n) \equiv \sum_{\text{all } k} \frac{1}{\eta_n (\zeta_k - \eta_n)^p} = \left(\frac{1}{\eta_n} \right) \sum_{\text{all } k} \frac{1}{(\zeta_k - \eta_n)^p} \equiv \frac{1}{\eta_n} \tilde{U}_p(n), \tag{22}$$

where

$$\tilde{U}_p(n) \equiv \sum_{\text{all } k} \frac{1}{(\zeta_k - \eta_n)^p}. \tag{23}$$

The related quantity where we sum over the k values corresponding to odd states, namely

$$\tilde{T}_p(n) \equiv \sum_{\text{all } k} \frac{1}{(\eta_k - \zeta_n)^p} \tag{24}$$

can be obtained by using the definition in equation (21) to write

$$\tilde{T}_p(n) = \zeta_n T_p(n) + T_{p-1}(n). \tag{25}$$

For completeness, we recall from [4] that for the quantum bouncer system constraints on sums were of the form

$$S_p(n) \equiv \sum_{k \neq n} \frac{1}{(\zeta_k - \zeta_n)^p}. \tag{26}$$

We will focus on evaluation of the $T_p(n)$ and $U_p(n)$, noting that it is straightforward to obtain the related $\tilde{T}_p(n)$, $\tilde{U}_p(n)$ for comparison to $S_p(n)$, using equations (22) and (25).

While not formally a sum rule, we note that the completeness relation for dipole matrix elements can be written as

$$\sum_{k \neq n} |\langle n|z|k \rangle|^2 + \langle n|z|n \rangle = \sum_{\text{all } k} |\langle n|z|k \rangle|^2 = \langle n|z^2|n \rangle \quad (27)$$

and that because of the parity of the potential the ‘diagonal’ term is in fact zero. While not a sum rule in the classic sense, it will also provide novel constraints on the A_i and A_i' zeros.

For the sum rules in equations (17)–(20) and (27), we can now fix a state of definite parity, either $\psi_n^{(+)}(z)$ or $\psi_n^{(-)}(z)$, and then sum over the states of opposite parity, namely the $\psi_k^{(-)}(z)$ or $\psi_k^{(+)}(z)$, respectively. In this way, we obtain two different constraints for each quantum-mechanical sum rule.

For example, starting with the TRK sum rule in equation (17) we find the relations

$$T_5(n) \equiv \sum_{\text{all } k} \frac{1}{\eta_k(\eta_k - \zeta_n)^5} = \frac{1}{4} = \left(\frac{1}{\eta_n}\right) \sum_{\text{all } k} \frac{1}{(\zeta_k - \eta_n)^5} \equiv U_5(n), \quad (28)$$

by using odd ($\psi_n^{(-)}$) and even ($\psi_n^{(+)}$) states, respectively. For comparison, we note that the constraint arising in this case for the quantum bouncer is

$$S_3(n) = \sum_{k \neq n} \frac{1}{(\zeta_k - \zeta_n)^3} = \frac{1}{4}. \quad (29)$$

From the momentum-completeness sum rule in equation (18), we use the evaluation of the \hat{p}^2 operator from equation (13) and find

$$T_4(n) = \sum_{\text{all } k} \frac{1}{\eta_k(\eta_k - \zeta_n)^4} = \frac{\zeta_n}{3} \quad (30)$$

$$U_4(n) = \left(\frac{1}{\eta_n}\right) \sum_{\text{all } k} \frac{1}{(\zeta_k - \eta_n)^4} = \frac{\eta_n}{3}, \quad (31)$$

while the corresponding sum rule constraint for the bouncer is

$$S_3(n) = \sum_{k \neq n} \frac{1}{(\zeta_k - \zeta_n)^2} = \frac{\zeta_n}{3}. \quad (32)$$

For the sum rule in equation (20), the fact that $[V'(z)]^2 = (\pm F)^2 = F^2$ for both positive and negative values of z , yields

$$T_2(n) = \sum_{\text{all } k} \frac{1}{\eta_k(\eta_k - \zeta_n)^2} = 1 = \left(\frac{1}{\eta_n}\right) \sum_{\text{all } k} \frac{1}{(\zeta_k - \eta_n)^2} = U_2(n). \quad (33)$$

The convergence of these sums is clear since the large k behavior of the $\zeta_k \sim k^{2/3}$ implies that each term scales as $k^{-4/3}$. Thus, $p = 2$ is the smallest power which will lead to a convergent sum rule. For the case of the quantum bouncer, this sum rule did not converge.

For the sum rule in equation (19) we require the value of $V''(z)$. Given the cusp in the definition of $V(z)$, we find that $V''(z) = 2F\delta(z)$ so that the right-hand side of equation (19) becomes

$$\frac{\hbar^4 F}{m^2} |\psi_n^{(\pm)}(0)|^2. \quad (34)$$

We can then use the results of equation (9) and immediately see that

$$T_3(n) = \sum_{\text{all } k} \frac{1}{\eta_k(\eta_k - \zeta_n)^3} = 0 \quad (35)$$

$$U_3(n) = \left(\frac{1}{\eta_n}\right) \sum_{\text{all } k} \frac{1}{(\zeta_k - \eta_n)^3} = \frac{1}{2}, \tag{36}$$

and note that the form of the right-hand side of this sum-rule constraint varies in form between the odd and even states. The only other case of which we are aware where the *force times momentum* sum rule gives a similar result, namely where the sum rule depends on the wavefunction at the origin, is for the Coulomb problem [15]. For that system, we have $\nabla^2 V(\mathbf{r}) = -e\delta(\mathbf{r})$ and the sum rule gives a non-zero result for *S*-wave ($l = 0$ states) only.

To evaluate the constraint arising from the z -completeness relation in equation (27), we require the expectation values of z^2 in the even and odd states. These can be derived by using the integral in equation (A.9) to obtain

$$\langle \psi_n^{(-)} | z^2 | \psi_n^{(-)} \rangle = \rho^2 \left(\frac{8\zeta_n^2}{15}\right) \quad \text{and} \quad \langle \psi_n^{(+)} | z^2 | \psi_n^{(+)} \rangle = \rho^2 \left(\frac{8\eta_n^2}{15} + \frac{1}{5\eta_n}\right), \tag{37}$$

where we once again notice the difference in form between the results for the two parities. Using these results, we find the following sum rules:

$$T_6(n) = \sum_{\text{all } k} \frac{1}{\eta_k(\eta_k - \zeta_n)^6} = \frac{2\zeta_n^2}{15} \tag{38}$$

$$U_6(n) = \left(\frac{1}{\eta_n}\right) \sum_{\text{all } k} \frac{1}{(\zeta_k - \eta_n)^6} = \frac{2\eta_n^2}{15} + \frac{1}{20\eta_n}. \tag{39}$$

The corresponding result for the quantum bouncer [4] has a non-zero ‘diagonal’ term, as in equation (27), which leads to the result

$$S_4 = \sum_{k \neq n} \frac{1}{(\zeta_k - \zeta_n)^4} = \frac{\zeta_n^2}{45}. \tag{40}$$

It has been stressed [2] that the form of the standard second-order perturbation theory result, namely

$$E_n^{(2)} = \sum_{k \neq n} \frac{|\langle n | \bar{V}(x) | k \rangle|^2}{(E_n^{(0)} - E_k^{(0)})}, \tag{41}$$

can also be thought of as an energy-weighted sum rule. Jackiw [16] discussed energy-difference weighted sum rules, containing factors such as $(E_k - E_n)^p$ with negative values of p . This concept was applied in [4] to obtain another independent constraint on the $S_p(n)$ for the quantum bouncer by considering the perturbing effect of an additional constant force (linear field) via the Stark effect.

The Stark effect for the symmetric linear potential has recently been discussed [8] where a straightforward expansion of the exact eigenvalue condition was shown to lead to closed-form expressions for the second-order energy shifts. If the perturbing potential is defined as $\bar{V}(z) = \bar{F}z$, then the results for the Stark shifts for the odd- and even-parity states respectively are found to be

$$E_n^{(-,2)} = -\frac{7}{9} \left(\frac{\bar{F}}{F}\right)^2 E_n^{(-)} \quad \text{and} \quad E_n^{(+,2)} = -\frac{5}{9} \left(\frac{\bar{F}}{F}\right)^2 E_n^{(+)}. \tag{42}$$

Using the expression in equation (41), we find that the second-order shifts given by perturbation theory are

$$E_n^{(-,2)} = -4 \left(\frac{\bar{F}}{F} \right)^2 \mathcal{E}_0 \left[\sum_{\text{all } k} \frac{1}{\eta_k (\eta_k - \zeta_n)^7} \right] \tag{43}$$

$$E_n^{(+,2)} = -4 \left(\frac{\bar{F}}{F} \right)^2 \mathcal{E}_0 \left[\sum_{\text{all } k} \frac{1}{\eta_n (\zeta_k - \eta_n)^7} \right], \tag{44}$$

which gives two new constraints

$$T_7(n) = \sum_{\text{all } k} \frac{1}{\eta_k (\eta_k - \zeta_n)^7} = + \frac{7\zeta_n}{36} \tag{45}$$

$$U_7(n) = \left(\frac{1}{\eta_n} \right) \sum_{\text{all } k} \frac{1}{(\zeta_k - \eta_n)^7} = + \frac{5\eta_n}{36}, \tag{46}$$

which can be compared to the the quantum bouncer

$$S_5(n) = \sum_{k \neq n} \frac{1}{(\zeta_k - \zeta_n)^5} = \frac{\zeta_n}{36}. \tag{47}$$

Our earlier discussion of sum rules for the quantum bouncer [4] allowed for a systematically calculable hierarchy of constraints on sums of inverse powers of $(\zeta_k - \zeta_n)$. This was made possible by repeated use of the commutation relation $[x^q, \hat{p}] = iq\hbar x^{q-1}$ to recursively obtain sums over matrix elements for higher and higher moments. For the symmetric potential, where matrix elements of odd powers of z vanish, that connection is lost and we know of no strategy to generate all of the $T_p(n)$ and $U_p(n)$ in a systematic way. We can, however, make use of the two relations

$$\sum_{\text{all } k} \langle n|x^q|k\rangle \langle k|x|n\rangle = \langle n|x^{q+1}|n\rangle \tag{48}$$

$$\sum_{\text{all } k} (E_k - E_n) \langle n|x^q|k\rangle \langle k|x|n\rangle = q \left(\frac{\hbar^2}{2m} \right) \langle n|x^{q-1}|n\rangle, \tag{49}$$

for q odd to generate an infinite number of new constraints on inverse powers of $(\eta_n - \zeta_k)$ similar to the ones derived already, requiring only the expectation values on the right-hand sides, which can in turn be evaluated using the recursion relations in appendix B.

The sum rules involving dipole matrix elements for the symmetric linear potential, using equations (14) and (15), give constraints on sums of inverse powers of $(\eta_k - \zeta_n)$. In order to obtain constraints on differences of just the zeros of $Ai'(\zeta)$ separately, namely the $(\eta_k - \eta_n)$, we need to consider matrix elements which are non-vanishing for even-even states. For example, because of the parity constraints in the symmetric linear potential, the so-called monopole sum rule [17]

$$\sum_{k \neq n} (E_k - E_n) |\langle n|z^2|k\rangle|^2 = \frac{2\hbar^2}{m} \langle n|z^2|n\rangle \tag{50}$$

will connect only odd-odd and even-even states; in this case the constraint that $k \neq n$ is indeed required. For the odd states, the corresponding constraint on the ζ_n was found in [4] to be

$$S_7(n) = \sum_{k \neq n} \frac{1}{(\zeta_k - \zeta_n)^7} = \frac{\zeta_n^2}{270}. \tag{51}$$

For the even–even case, we can use the new matrix element result in equation (A.13) to evaluate

$$\langle \psi_n^{(+)} | z^2 | \psi_k^{(+)} \rangle = -\frac{12(\eta_n + \eta_k)}{\sqrt{\eta_n \eta_k} (\eta_n - \eta_k)^4}, \quad (52)$$

which gives a more complicated constraint, namely

$$\sum_{k \neq n} \frac{(\eta_n + \eta_k)^2}{\eta_n \eta_k (\eta_n - \eta_k)^7} = \frac{1}{36} \left(\frac{8\eta_n^2}{15} + \frac{1}{5\eta_n} \right). \quad (53)$$

Once again, we have checked all of these results numerically using Mathematica[®].

The new classes of constraints on the zeros of A_i and A_i' derived here, from application of sum rules for the symmetric linear potential, are seen to be qualitatively similar to those obtained from the parity-restricted version of this potential, namely the quantum bouncer. In contrast, the nature of the mathematical relations dictated by sum rules applied to the parity-restricted version of the harmonic oscillator are qualitatively very different, as we will see in section 5, after first reviewing sum rules in the standard oscillator system.

4. Review of sum rules for the harmonic oscillator

Before examining the parity-restricted version of the harmonic oscillator, we briefly review the solutions for the the familiar oscillator potential, as well as the structure of the quantum mechanical sum rules for this system. The solutions for the Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_n(x)}{dx^2} + \frac{1}{2} m \omega^2 x^2 \psi_n(x) = E_n \psi_n(x) \quad (54)$$

can be written in the form

$$\psi_n(x) = \frac{c_n}{\sqrt{\beta}} H_n(y) e^{-y^2/2}, \quad \text{where} \quad c_n = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} \quad (55)$$

and

$$x = \beta y \quad \text{and} \quad \beta \equiv \sqrt{\frac{\hbar}{m\omega}}, \quad (56)$$

with y dimensionless and the $H_n(y)$ are the Hermite polynomials. The corresponding energy eigenvalues are

$$E_n = (n + 1/2)\hbar\omega \quad \text{or} \quad \epsilon_n \equiv \frac{2E_n}{\hbar\omega} = 2n + 1, \quad (57)$$

with $n = 0, 1, \dots$ so that the differential equation in dimensionless form can be written as

$$\psi_n''(y) = (y^2 - \epsilon_n)\psi_n. \quad (58)$$

The solutions have parity given by $P_n = (-1)^n$ and the expectation values of any odd power of x vanishes, so that, for example, $\langle n | x^{2p+1} | n \rangle = 0$.

Both x and \hat{p} can be written in terms of raising and lowering operators, \hat{A} and \hat{A}^\dagger , and hence the multipole matrix elements exhibit an exceptionally simple structure leading to absolute selection rules. For example, we have from standard textbooks the relations

$$\langle n | x | k \rangle = \frac{\beta}{\sqrt{2}} \{ \delta_{n,k-1} \sqrt{k} + \delta_{n,k+1} \sqrt{k+1} \} \quad (59)$$

$$\langle n | x^2 | k \rangle = \frac{\beta^2}{2} \{ \delta_{n,k-2} \sqrt{k(k-1)} + \delta_{n,k} (2k+1) + \delta_{n,k+2} \sqrt{(k+1)(k+2)} \} \quad (60)$$

$$\langle n|x^3|k\rangle = \frac{\beta^3}{2\sqrt{2}} \left\{ \delta_{n,k-3} \sqrt{k(k-1)(k-2)} + 3\delta_{n,k-1} k^{3/2} + 3\delta_{n,k+1} (k+1)^{3/2} + \delta_{n,k+3} \sqrt{(k+1)(k+2)(k+3)} \right\}. \tag{61}$$

These, and similar expressions for matrix elements of powers \hat{p} , imply that all of the familiar sum rules discussed above will be ‘super-convergent’, namely that the relevant infinite sums will actually be saturated by a finite number of terms, and hence satisfied in a trivial way. We will find that the situation is dramatically different in the case of the oscillator restricted to the half-line, at least for the matrix elements of odd values of x , and that is the subject of the next section. The matrix element relations for even powers of x , including equation (60), will still be relevant for the restricted oscillator case with minor relabeling.

5. The parity-restricted harmonic oscillator

The solutions to the quantum mechanical problem of a particle in the potential in equation (3) are easily obtained from the odd-parity solutions in equation (55). In dimensionless notation, we have

$$\tilde{\psi}_n(y) = \begin{cases} \sqrt{2}\psi_{2n+1}(y) & \text{for } y \geq 0 \\ 0 & \text{for } y \leq 0, \end{cases} \tag{62}$$

where $n = 0, 1, 2, \dots$ for the ‘half’-SHO states $\tilde{\psi}_n(y)$ associated with the odd solutions of the oscillator, and an appropriate change in overall normalization. We will henceforth use integrals over either the dimensional x or dimensionless y variable as deemed most useful. We note for future reference that the derivatives of the solutions at the origin necessary for matrix element calculations are given by

$$\tilde{\psi}'_n(0) = \sqrt{2}c_{2n+1} H'_{2n+1}(0) = \frac{(-1)^n 2}{\sqrt{(2n+1)!} \sqrt{\pi}} (2n+1)!! = \frac{(-1)^n 2}{2^n n!} \sqrt{\frac{(2n+1)!}{\sqrt{\pi}}} \tag{63}$$

and

$$[\tilde{\psi}'_n(0)]^2 = \frac{4}{2^{2n} (n!)^2} \frac{(2n+1)!!}{\sqrt{\pi}} = \frac{1}{\sqrt{\pi}} \left[\frac{4(2n+1)!}{2^{2n} (n!)^2} \right] = \frac{D_n}{\sqrt{\pi}}, \tag{64}$$

where

$$D_n \equiv \frac{4(2n+1)!}{2^{2n} (n!)^2}. \tag{65}$$

Using the Stirling approximation, $n! \sim \sqrt{2\pi n} (n/e)^n$, we have for large n

$$D_n \rightarrow 8\sqrt{\frac{n}{\pi}}, \tag{66}$$

which will be useful in examining the semi-classical limit.

The quantized energies for the ‘half’-SHO are then given by $\tilde{E}_n = E_{2n+1} = (2n+3/2)\hbar\omega$ or $\tilde{\epsilon}_n = 4n+3$. The $\tilde{\psi}_n(y)$ form an orthogonal set which can be seen explicitly by using the recursion relation derived for oscillator solutions in appendix B. Using $f(y) = 1$ in equation (B.8), we find that

$$(\tilde{\epsilon}_n - \tilde{\epsilon}_m)^2 \int_0^\infty \tilde{\psi}_n(y)\tilde{\psi}_m(y) dy = 0, \tag{67}$$

so that $\langle \tilde{\psi}_m | \tilde{\psi}_n \rangle = 0$ if $n \neq m$.

For the important dipole matrix elements, we use $f(y) = y$, so that $f'(0) = 1$ and find that

$$\langle \tilde{\psi}_m | y | \tilde{\psi}_n \rangle = \int_0^\infty y \tilde{\psi}_n(y) \tilde{\psi}_m(y) dy = -\frac{\tilde{\psi}'_n(0)\tilde{\psi}'_m(0)}{2[4(n-m)^2 - 1]} \tag{68}$$

since $\tilde{\epsilon}_n = 4n + 3$.

For the special case of $n = m$, the expectation values in the state $\tilde{\psi}_n$ are therefore given by

$$\langle \tilde{\psi}_n | x | \tilde{\psi}_n \rangle = \frac{D_n}{2\sqrt{\pi}}\beta \longrightarrow \frac{4\sqrt{n}}{\pi}\beta \tag{69}$$

in the large n limit. We can confirm this by using the classical (WKB-like) probability distribution for the ‘half’-SHO, namely

$$P_{CL}^{(n)}(x) = \frac{2}{\pi} \frac{1}{\sqrt{A^2 - x^2}}, \quad \text{where } 0 \leq x \leq A_n, \tag{70}$$

where the upper classical turning point, A_n , is given by

$$\frac{1}{2}m\omega^2 A_n^2 = E_n = \hbar\omega(2n + 3/2) \quad \text{or} \quad A_n = \beta\sqrt{4n + 3}. \tag{71}$$

The classical expectation value is then

$$\langle n | x | n \rangle_{CL} \equiv \int_0^{A_n} x P_{CL}^{(n)}(x) dx = \frac{2A_n}{\pi} = \frac{2\sqrt{4n + 3}}{\pi} \beta \longrightarrow \left(\frac{4\sqrt{n}}{\pi}\right) \beta \tag{72}$$

for large n , which agrees with equation (69).

The dipole matrix elements in equation (68) are clearly very different from the ‘full’-SHO case, with each state being connected to all of the others in a very simple form, proportional to the derivative of the wavefunction at the origin for each state, and with an ‘energy denominator’ factor. This is the only example of a dipole matrix element in a model 1D system of which we are aware for which the diagonal ($n = m$) and off-diagonal ($n \neq m$) cases can be written with the same simple expression. The corresponding sum rules will then be realized in a completely different manner than the super-convergent form for the more familiar oscillator.

For example, the TRK sum rule in equation (17) gives the constraint

$$D_n \sum_{k \neq n} \frac{(k - n)D_k}{[4(n - k)^2 - 1]^2} = \pi, \tag{73}$$

where the D_n are given in equation (65). In a similar way, the x -completeness relation of equation (27) gives

$$D_n \sum_{k \neq n} \frac{D_k}{[4(n - k)^2 - 1]^2} = (8n + 6)\pi, \tag{74}$$

where we use the fact that

$$\langle \tilde{\psi}_n | y^2 | \tilde{\psi}_n \rangle = (2n + 3/2), \tag{75}$$

making use of the matrix element in equation (60) with a suitable relabeling. One can then combine equations (73) and (75) to obtain the constraint

$$D_n \sum_{k \neq n} \frac{kD_k}{[4(n - k)^2 - 1]^2} = (4n + 1)(2n + 1)\pi. \tag{76}$$

Looking at the n and k dependence of the dipole matrix elements, one can confirm that the sum rules in equations (19) and (20) which depend on derivatives of $V(x)$ are not convergent; this result is consistent with the nature of the discontinuous potential.

Matrix elements involving even powers of x can be written in terms of the results for the ‘full’-SHO and have the same simple ‘nearby neighbor’ selection rule structure. For example, a simple relabeling of equation (60) gives

$$\langle \tilde{\psi}_n | y^2 | \tilde{\psi}_k \rangle = \frac{1}{2} \{ \delta_{n,k-1} \sqrt{(2k+1)(2k)} + \delta_{n,k} (4k+3) + \delta_{n,k+1} \sqrt{(2k+2)(2k+3)} \}, \quad (77)$$

and the monopole sum rule in equation (50) is saturated by a finite number of terms. Matrix element relations using odd powers of x , such as those in equations (48) and (49) give increasing complicated relations involving the $D_{k,n}$ since the matrix elements of x^{2q+1} all are proportional to $\langle \tilde{\psi}_n | x | \tilde{\psi}_k \rangle$. For example, using the recursion relation in equation (B.8), we find that

$$\begin{aligned} \langle \tilde{\psi}_n | y^3 | \tilde{\psi}_k \rangle &= \frac{-6(2n+2k+3)}{[4(n-k)^2-9]} \langle \tilde{\psi}_n | y | \tilde{\psi}_k \rangle \\ &= \frac{-3(2n+2k+3)}{[4(n-k)^2-9][4(n-k)^2-1]} \left(\frac{\tilde{\psi}'_n(0)\tilde{\psi}'_k(0)}{2} \right). \end{aligned} \quad (78)$$

One can continue to generate increasingly complex constraints by use of equations (48) and (49) for the non-trivial case of matrix elements of the odd powers of x .

The realization of the sum rules for the parity-restricted version of the oscillator are completely different than the trivial manner in which they are satisfied for the ordinary oscillator system and generate an infinite number of constraints on the D_n .

6. Classical versus quantum mechanical results

We have seen that some of the matrix element expressions and/or sum rules for the symmetric linear potential yield identical results when considering both the even and odd cases, with only the substitution $\zeta_n \leftrightarrow \eta_n$ required: the virial theorem result in equation (12) and the TRK, momentum completeness and *force-squared* sum rules in equations (28), (30), (31) and (33). For others, however, such as the second-moment expectation values in equation (37) or the *force times momentum* result one finds slightly different results.

To examine these small differences, we will consider the classical underpinnings of some of the results which arise in the evaluation of expectation values. By generalizing the recursion relation derived by Goodmanson [10], in appendix B one can generate the expectation values and off-diagonal matrix elements of any power of z .

For example, from [4] we know that expectation values of z^p for the quantum bouncer solutions are given by

$$\langle n | y | n \rangle = \frac{2\zeta_n}{3} \quad (79)$$

$$\langle n | y^2 | n \rangle = \frac{8\zeta_n^2}{15} \quad (80)$$

$$\langle n | y^3 | n \rangle = \frac{16\zeta_n^3}{35} + \frac{3}{7} \quad (81)$$

$$\langle n | y^4 | n \rangle = \frac{128\zeta_n^4}{315} + \frac{80\zeta_n}{63} \quad (82)$$

$$\langle n | y^5 | n \rangle = \frac{256\zeta_n^5}{693} + \frac{1808\zeta_n^2}{3003}, \quad (83)$$

where $y = z/\rho$ and we only show the dimensionless results. Each result has a highest-order term of order $(\zeta_n)^p$, followed by the sub-leading terms of order ζ_n^{p-3k} , if present at all. Using

the large- n expansion of the ζ_n in equation (7), we see that the sub-leading terms are a factor of $(\zeta_n)^{-3k} \sim n^{-k}$ smaller and so become negligible in the classical limit. This suggests that the leading terms are indeed what one would expect from a purely classical probability density.

To confirm this, we note that for the quantum bouncer we have

$$P_{CL}^{(n)}(z) = \frac{1}{2\sqrt{A_n(A_n - z)}}, \tag{84}$$

where A_n is the upper classical turning point, defined by $E_n = FA_n$. If we equate total energy with the quantum mechanical result $E_n = (F\rho)\zeta_n$ and write $A_n = \rho\zeta_n$, the classical probability density reduces to

$$P_{CL}^{(n)}(z) = \frac{1}{2\rho\sqrt{\zeta_n(\zeta_n - z/\rho)}}. \tag{85}$$

We briefly discuss, in appendix C, how this classical distribution can also be extracted directly from the large n limit of the exact quantum solutions.

The expectation values of moments of position are then given by

$$\begin{aligned} \langle n|z^p|n\rangle_{CL} &= \int_0^{A_n} z^p P_{CL}^{(n)}(z) dz \\ &= \rho^p \int_0^{\zeta_n} \frac{z^p}{2\sqrt{\zeta_n(\zeta_n - z)}} dz \\ &= \frac{\rho^p \zeta_n^p}{2} \int_0^1 \frac{y^p}{\sqrt{1-y}} dy \\ &= \frac{(\rho\zeta_n)^p}{2} B(p+1, 1/2) \\ &= \frac{(\rho\zeta_n)^p}{2} \frac{\Gamma(1+p)\Gamma(1/2)}{\Gamma(p+3/2)}, \end{aligned} \tag{86}$$

and this expression agrees with the leading-order terms in equations (79)–(83) up through $p = 5$. Using the recursion relation of Goodmanson, reviewed and extended in the appendix, we can assume generally that the behavior of the leading term for the expectation values can be written as $\langle n|x^p|n\rangle = A_n^p$ and the recursion relation requires that

$$A_n^q = \frac{2q\zeta_n}{(2q+1)} A_n^{q-1} \quad \text{or} \quad A_n^p = \frac{2^p p!}{(2p+1)!!} \zeta_n^p, \tag{87}$$

which agrees with the classical result in equation (86) for all p values.

For the symmetric linear potential, the expectation values for odd powers of x vanish, but the integrals in equations (79)–(83) are still useful. For example, for the expectation value of $V(z) = F|z|$, we require the result in equation (79). Moreover, because of the piecewise continuous definition of the wavefunctions in equations (4) and (6), the integrals obtained by using the recursion relations in appendix B are necessarily defined over the interval $(0, \infty)$ and then extended over all space, so intermediate results for integrals over the half-line which eventually vanish due to parity constraints can still be useful.

To compare the leading and sub-leading contributions to integrals used for the expectation values for odd and even states, we can compare the results in equations (79)–(83) to similar results for the even states. These can be defined by using the states in equation (6), integrated over positive values of z and normalized as for the quantum bouncer. For those cases we find

$$\langle n|y|n\rangle = \frac{2\eta_n}{3} \tag{88}$$

$$\langle n|y^2|n\rangle = \frac{8\eta_n^2}{15} + \frac{1}{4\eta_n} \tag{89}$$

$$\langle n|y^3|n\rangle = \frac{16\eta_n^3}{35} + \frac{3}{5} \tag{90}$$

$$\langle n|y^4|n\rangle = \frac{128\eta_n^4}{315} + \frac{64\eta_n}{45} \tag{91}$$

$$\langle n|y^5|n\rangle = \frac{256\eta_n^5}{693} + \frac{272\eta_n^2}{99} + \frac{6}{11\eta_n}. \tag{92}$$

We note that the leading terms in each case (and quite generally for all values of p , using a recursion relation argument as above) are identical (with $\zeta_n \leftrightarrow \eta_n$), but that the next-to-leading orders reflect differences between the classical and quantum probability densities. These differences vanish in the large n limit.

In the context of the ‘half’-SHO, we have already noted that there can be similar agreement between the exact quantum-mechanical expectation value of x in equation (69) and the corresponding classical result in equation (72) in the large n limit. One can use the recursion relations in equation (B.8) to obtain the highest-order terms in the expectation values of x^p , and one again finds agreement with the semi-classical results for large n . For example, the classical result is

$$\langle n|x^p|n\rangle_{CL} = \frac{2}{\pi} \int_0^{A_n} \frac{x^p}{\sqrt{A_n^2 - x^2}} dx = \frac{2(A_n)^p}{\pi} \int_0^1 \frac{y^p dy}{\sqrt{1 - y^2}} = \frac{(A_n)^p}{\sqrt{\pi}} \frac{\Gamma((1 + p)/2)}{\Gamma(1 + p/2)}. \tag{93}$$

Given that traditional sum rules involve transition matrix elements, there is no reason to expect that semi-classical probability arguments will provide any useful information on their evaluation. One important exception, however, is the form of the second-order perturbation theory result for the energy, as in equation (41), which is of the form of an energy-difference weighted sum rule. In that special case, semi-classical expressions for the quantized energy, such as the WKB approximation, can sometimes provide guidance on the form of the energies, at least in the large n limit.

An example of such a connection is the use of approximate WKB-type methods in the evaluation of first-order perturbation theory results using classical probability densities, as in [18]. More surprisingly, it has been pointed out that WKB energy quantization methods can give the correct large n behavior of the second-order energy shift due to the Stark effect in two familiar model systems, the harmonic oscillator and infinite well [19]. This approach was used in [8] where the exact result for the second-order energy shift due to a constant external field for the symmetric linear potential was derived for the first time, giving the results in equation (42). The WKB prediction for this case is given by the quantization condition

$$\sqrt{2m} \int_{A_-}^{A_+} \sqrt{E_n - (F|z| + \bar{F}z)} dz = (n + 1/2)\hbar\pi, \tag{94}$$

where $n = 0, 1, 2, \dots$ and the classical turning points are $A_{\pm} = \pm E_n/(F \pm \bar{F})$. The WKB prediction for the energies are then

$$E_n = E_n^{(0)} \left(1 - \frac{\bar{F}^2}{F^2} \right)^{2/3} \approx E_n^{(0)} \left(1 - \frac{2}{3} \left(\frac{\bar{F}}{F} \right)^2 + \dots \right), \tag{95}$$

where $E_n = \mathcal{E}_0(3\pi(n + 3/4)/2)^{2/3}$ is the zero-field WKB approximation, which agrees with the exact results in equation (7) for large n . This implies that the first-order Stark shift vanishes

(as it must by symmetry) and that the second-order terms are

$$E_n^{(2)} = -\frac{6}{9} \left(\frac{\bar{F}}{F}\right)^2 E_n^{(0)}. \tag{96}$$

As pointed out in [8], this semi-classical result brackets the two exact quantum mechanical expressions for the even and odd states in equation (42), giving it as the ‘average’ effect.

Prompted by this partial success, we wish to examine to what extent a similar WKB-type analysis will give reliable answers for the first- and second-order energy shifts due to the Stark effect for the ‘half’-SHO discussed above. We first note that the WKB result for the energy eigenvalues for the potential in equation (3) without an external field are given by

$$\sqrt{2m} \int_0^{A_n} \sqrt{E_n - m\omega^2 x^2/2} dx = (n + C_L + C_R)\hbar\pi, \tag{97}$$

where C_L, C_R are the appropriate matching constants for an infinite wall and ‘linear’ potential respectively, given by $C_L = 1/2$ and $C_R = 1/4$, respectively. Evaluating the integral, the WKB prediction is then given by $E_n = (2n + 3/2)\hbar\omega$, reproducing the exact result.

The corresponding expression including a perturbing linear field, $\bar{V}(x) = \bar{F}x$, is then

$$\sqrt{2m} \int_0^{A_n^{(+)}} \sqrt{E - m\omega^2 x^2/2 - \bar{F}x} dx = (n + 3/4)\hbar\pi, \tag{98}$$

where the upper turning point is given by energy conservation to be

$$A_n^{(+)} = \frac{\sqrt{2m\omega^2 E_n + \bar{F}^2} - \bar{F}}{m\omega^2}. \tag{99}$$

The integral can be done in closed form, but we only require the result expanded to second order in \bar{F} , which gives

$$\frac{\pi}{2} \sqrt{\frac{m}{m\omega^2}} \left[E_n - \frac{2}{\pi} \sqrt{\frac{2E_n}{m\omega^2}} \bar{F} + \frac{\bar{F}^2}{2m\omega^2} \right] = (n + 3/4)\hbar\pi. \tag{100}$$

This can be rationalized to give the simple quadratic equation

$$E_n = R_n \pm \sqrt{R_n^2 - Z_n^2}, \tag{101}$$

where

$$Z_n \equiv \frac{\bar{F}^2}{2m\omega^2} \quad \text{and} \quad R_n = Z_n + \frac{4\bar{F}^2}{\pi^2 m\omega^2}. \tag{102}$$

Solving for E_n , again as a series in \bar{F} , we find that

$$E_n^{(0)}(WKB) = (2n + 3/2)\hbar\omega \tag{103}$$

$$E_n^{(1)}(WKB) = \frac{2\bar{F}}{\pi} \sqrt{\frac{2E_n^{(0)}}{m\omega^2}} \tag{104}$$

$$E_n^{(2)}(WKB) = \left(-\frac{1}{2} + \frac{4}{\pi^2}\right) \frac{\bar{F}^2}{m\omega^2}. \tag{105}$$

The zero-order result is the standard WKB prediction noted above, while the first-order expression coincides with first-order perturbation theory (using the matrix element in equation (69) in the large n limit.

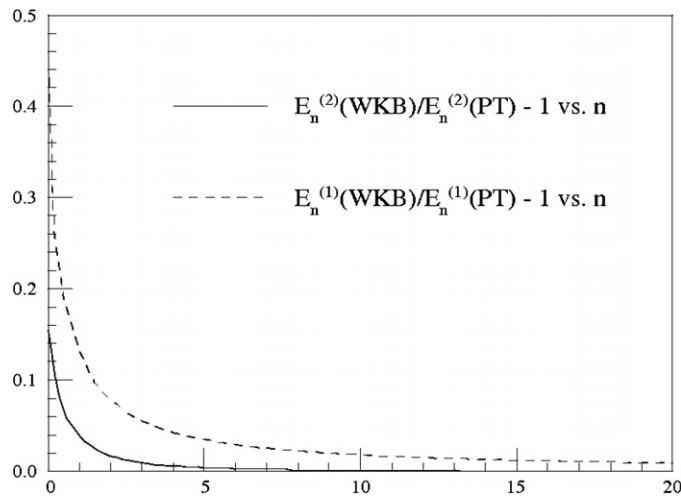


Figure 1. Comparison of the WKB estimate (WKB) of the first- and second-order energies for the Stark effect (from equations (104) and (105)) versus the exact results from perturbation theory (PT). The quantity $E_n^{(1,2)}(WKB)/E_n^{(1,2)}(PT) - 1$ is shown as dashed (first-order) and dashed (second-order), respectively.

The second-order result is more interesting. The exact quantum mechanical result for the second-order Stark effect for the ordinary harmonic oscillator is $E_n^{(2)} = -\bar{F}^2/2m\omega^2$ which is most easily obtained by a simple change of variables in the original Schrödinger equation, and trivially confirmed in second-order perturbation theory, using the matrix elements in equation (59). For the ‘half’-SHO, the WKB prediction is still a constant negative shift, the same for all states, but with a non-trivially different coefficient. We can find no simple way to extract the exact second-order result from a direct solution of the differential equation, but the second-order perturbation theory expression in equation (41) can be evaluated numerically using the dipole matrix elements in equation (68).

To compare the first- and second-order predictions from the WKB approach with the exact results from first- and second-order PT, we plot the differences between the WKB and PT methods in figure 1, as a function of the quantum number n . As mentioned above, the first-order predictions in both approaches agree in the large n limit, which we have demonstrated here analytically. We note the more interesting result that the simple expression in equation (105) gives the correct large n behavior of the second-order Stark shifts for the ‘half’-SHO problem, reproducing a non-trivial numerical factor which would otherwise be difficult to extract.

We note that this is another example of where a WKB approach to the evaluation of the second-order Stark effect correctly predicts the large n behavior. This further justifies the discussion [19], where such an approach was used to systematically evaluate the second-order energy shifts due to an external field for general power-law potentials, $V_k(x) = V_0|x/a|^k$.

7. Conclusions and discussion

We have examined two cases of parity-related potentials, the quantum bouncer extended to the symmetric linear potential, and the harmonic oscillator reduced to the ‘half’-SHO, in order to probe the importance of the continuity of the potential on the convergence of

quantum mechanical sum rules. We have indeed seen that the smoothness of $V(x)$ has clear consequences on which sum rules will be realized, which in turn is closely related to the convergence properties of the individual matrix elements. For the symmetric linear potential, we find new constraints on the zeros of the derivative of the Airy function, but note that they are very similar in functional form to those derived from the quantum bouncer. On the other hand, the infinite set of constraints which arise from the ‘half’-SHO are qualitatively very different from the super-convergent sums found in the realization of sum rules for the more familiar oscillator.

The study of parity-related potentials is also motivated by the desire to find examples where there is a substantial overlap between the energies and wavefunctions (needed in the evaluation of matrix elements) of two quantum systems as they relate to sum rules. That connection is realized here by the fact that the odd states of a symmetric potential remain solutions of the parity-restricted version, so that all of the resulting energies and wavefunctions (save a trivial normalization) are still solutions of the parity-restricted partner potential.

Another class of quantum mechanical problems which has similar strong connections between the energy levels and wavefunctions are super-partner potentials [20], $V^{(-)}(x)$ and $V^{(+)}(x)$, in the context of supersymmetric quantum mechanics (SUSY-QM). In that case, the spectra of the two systems are identical, except for the zero-energy ground state ($E_0^{(-)} = 0$) of the first system, which is absent in the second. Another reason for us to consider the ‘half’-SHO potential in such detail is that it is easily extended to generate an appropriate $V^{(\pm)}(x)$ pair in SUSY-QM. For example, the potential

$$V^{(-)}(x) = \frac{1}{2}m\omega^2x^2 - \frac{3}{2}\hbar\omega \quad \text{for } x \geq 0 \tag{106}$$

has the energy spectrum $E_n^{(-)} = 2n\hbar\omega$ for $n = 0, 1, 2, \dots$ with the ground state wavefunction

$$\psi_0(x) = \frac{2x}{\sqrt{\beta^3}\sqrt{\pi}} e^{-(x/\beta)^2/2} \quad \text{for } x \geq 0, \tag{107}$$

and the remaining states given by equation (62).

Using this ground-state solution to form the super-potential, we find

$$W(x) = -\frac{\hbar}{\sqrt{2m}} \left(\frac{\psi_0'(x)}{\psi_0(x)} \right) = -\frac{\hbar}{\sqrt{2m}} \left(\frac{1}{x} - \frac{x}{\beta^2} \right), \tag{108}$$

allowing us to construct the super-partner potential

$$V^{(+)}(x) = \frac{1}{2}m\omega^2x^2 + \frac{2\hbar^2}{2mx^2} - \frac{1}{2}\hbar\omega. \tag{109}$$

This has the form of the radial equation for the three-dimensional harmonic oscillator with the special choice of the angular momentum quantum number $l = 1$ (giving the $l(l + 1) = 2$ factor in the centrifugal barrier term) and an overall constant shift in energy. Using standard results for the energy eigenvalues for that system, we find that

$$E_n^{(+)} = \hbar\omega \left(2n + l + \frac{3}{2} \right) - \frac{1}{2}\hbar\omega = 2\hbar\omega(n + 1), \tag{110}$$

for the relevant $l = 1$ case. One can also use standard textbook results to obtain the properly normalized solutions to be

$$\psi_n^{(+)}(x) = N_n x^2 e^{-(x/\beta)^2/2} L_n^{(3/2)}(x^2/\beta^2) \quad \text{with} \quad N_n = \sqrt{\frac{2^{k+3}k!}{\beta^5(2k+3)!!\sqrt{\pi}}}. \tag{111}$$

This is one example of many familiar super-partner potentials [20] which can be systematically studied in the context of quantum mechanics to probe the delicate interplay between energy level differences and matrix elements which must exist to guarantee the realization of the

infinite number of sum rules which one can generate using the simple procedures outlined here.

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Appendix A. Necessary integrals involving Airy function

In this appendix, we collect indefinite integrals of products of Airy functions, useful for normalizations, expectation values and matrix elements as first noted by Gordon [13] and Albright [14], adding one new result (equation (A.13)).

We then extend the recursion relation for general matrix elements of Airy functions, first derived by Goodmanson [10], necessary for both the even and odd states of the symmetric linear potential in appendix B and also generalize those recursion relations to the case of the harmonic oscillator problem, allowing one to evaluate matrix elements for the ‘half’-SHO problem.

We first assume two arbitrary linear combinations of the solutions of the Airy differential equation:

$$A(\zeta - \beta) = aAi(\zeta - \beta) + bBi(\zeta - \beta) \quad \text{and} \quad B(\zeta - \beta) = cAi(\zeta - \beta) + dBi(\zeta - \beta), \tag{A.1}$$

where

$$A''(\zeta - \beta) = (\zeta - \beta)A(\zeta - \beta) \quad \text{and} \quad B''(\zeta - \beta) = (\zeta - \beta)B(\zeta - \beta). \tag{A.2}$$

In the expressions below, when we refer to integrals of such solutions corresponding to different values of the ‘shift’, $\beta_1 \neq \beta_2$, we write A_1 for $A(\zeta - \beta_1)$ and B_2 for $B(\zeta - \beta_2)$.

Each of the indefinite integrals we need can be written in terms of four basic quantities, namely

$$F_1 = \{AB\} \tag{A.3}$$

$$F_2 = \{A'B - AB'\} \tag{A.4}$$

$$F_3 = \{A'B + AB'\} \tag{A.5}$$

$$F_4 = \{A'B'\}, \tag{A.6}$$

times polynomials in ζ and the appropriate values of β .

For the integrals involving solutions with the same ‘shift’, we have

$$\int AB \, d\zeta = (\zeta - \beta)F_1 - F_4 \tag{A.7}$$

$$\int \zeta AB \, d\zeta = \frac{1}{3}(\zeta^2 + \beta\zeta - 2\beta^2)F_1 + \frac{1}{6}F_3 - \frac{1}{3}(\zeta + 2\beta)F_4 \tag{A.8}$$

$$\int \zeta^2 AB \, d\zeta = \frac{1}{15}(3\zeta^3 + \beta\zeta^2 + 4\beta^2\zeta - 8\beta^3 - 3)F_1 + \frac{1}{15}(3c + 2\beta)F_3 - \frac{1}{15}(3\zeta^2 + 4\beta\zeta + 8\beta^2)F_4. \tag{A.9}$$

For integrals involving derivatives, we can modify one of the identities in Albright [14] to write for shifted solutions

$$\int A' B' d\zeta = -\frac{1}{3}(\zeta - \beta)^2 F_1 + \frac{1}{3} F_3 + \frac{1}{3}(\zeta - \beta) F_4. \tag{A.10}$$

Finally, for integrals with two different shifts ($\beta_1 \neq \beta_2$), we have results for $p = 0, 1$ from Gordon [13] and a new result derived here for $p = 2$. Recall that the T_i below will be constructed from the terms in equations (A.3)–(A.6) using $A_1 = A(\zeta - \beta_1)$ and $B_2 = B(\zeta - \beta_2)$:

$$\int A_1 B_2 d\zeta = \frac{1}{(\beta_2 - \beta_1)} F_2 \tag{A.11}$$

$$\int \zeta A_1 B_2 d\zeta = \frac{(\beta_1 + \beta_2 - 2\zeta)}{(\beta_1 - \beta_2)^2} F_1 + \left\{ \frac{\zeta}{(\beta_2 - \beta_1)} + \frac{2}{(\beta_2 - \beta_1)^3} \right\} F_2 + \frac{2}{(\beta_1 - \beta_2)^2} F_4 \tag{A.12}$$

$$\begin{aligned} \int \zeta^2 A_1 B_2 d\zeta = & \left[\frac{12(\beta_1 + \beta_2)}{(\beta_1 - \beta_2)^4} + \frac{2(-12 + (\beta_1 + \beta_2)(\beta_1 - \beta_2)^2)}{(\beta_1 - \beta_2)^4} \zeta - \frac{4}{(\beta_1 - \beta_2)^2} \zeta^2 \right] F_1 \\ & + \left[\frac{4(-6 + (\beta_1 + \beta_1)(\beta_1 - \beta_2)^2)}{(\beta_1 - \beta_2)^5} - \frac{12}{(\beta_1 - \beta_2)^3} \zeta - \frac{1}{(\beta_1 - \beta_2)} \zeta^2 \right] F_2 \\ & - \left[\frac{2}{(\beta_1 - \beta_2)^2} \right] F_3 + \left[\frac{24}{(\beta_1 - \beta_2)^4} + \frac{4}{(\beta_1 - \beta_2)^2} \zeta \right] F_4. \end{aligned} \tag{A.13}$$

Appendix B. Recursion relation for matrix elements of Airy functions and harmonic oscillator solutions

Goodmanson [10] derived a recursion relation relating the power-law matrix elements of solutions for the quantum bouncer problem, involving integrals of the form

$$R_p = \int_0^\infty \zeta^p Ai(\zeta - \zeta_n) Ai(\zeta - \zeta_m) d\zeta, \tag{B.1}$$

assuming that the solutions satisfied the boundary condition for the bouncer problem, namely that $Ai(-\zeta_n) = Ai(-\zeta_m) = 0$. One can easily repeat his analysis, not making that assumption, to find a more general recursion relation valid for integrals relevant for both the even and odd states of the symmetric linear potential. We can also repeat the analysis to obtain relations on matrix elements of the solutions of the harmonic oscillator, which will prove useful for the parity restricted ‘half’-SHO in section 5.

B.1. Recursion relations for Airy functions We begin by adopting the notation

$$A_n = A_n(\zeta) \equiv Ai(\zeta - \zeta_n), \quad \text{where } A_n'' = A_n''(\zeta) = (\zeta - \zeta_n) A_n, \tag{B.2}$$

and then assume a general $f(\zeta)$ as a well-behaved function, at least multiply differentiable and satisfying $\lim_{\zeta \rightarrow \infty} f(\zeta) Ai[\zeta]^2 = 0$. We will, in fact, use $f(\zeta) = \zeta^p$ to evaluate various matrix elements.

We start with the mathematical identity

$$\int_0^\infty [2f'(\zeta) A_n' A_m' - f''(\zeta) (A_n A_m)'] d\zeta = [2f'(\zeta) A_n' A_m' - f''(\zeta) (A_n A_m)']_0^\infty, \tag{B.3}$$

and then use integration by parts multiple times to isolate the $A_n(\zeta)A_m(\zeta)$ terms times derivatives of $f(\zeta)$ (on the left-hand side) and resulting surface terms (on the right-hand side). The resulting integral can be written in the form

$$I \equiv \int_0^\infty A_n A_m [f^{(iv)}(\zeta) - 4(\zeta - \zeta_{ave})f''(\zeta) - 2f'(\zeta) + (\zeta_n - \zeta_m)^2 f(\zeta)] d\zeta, \tag{B.4}$$

which can be shown to be equal to

$$\begin{aligned} I &= [2f'(\zeta)A'_n A'_m - f''(\zeta)(A_n A_m)']_0^\infty + [f'''(\zeta)A_n A_m]_0^\infty - [2A_n A_m(\zeta - \zeta_{ave})f'(\zeta)]_0^\infty \\ &\quad - [(\zeta_n - \zeta_m)(A'_n A_m - A_n A'_m)f(\zeta)]_0^\infty \\ &= -2f'(0)A'_n(0)A'_m(0) + f''(0)[A'_n(0)A_m(0) + A_n(0)A'_m(0)] - f'''(0)A_n(0)A_m(0) \\ &\quad - 2A_n(0)A_m(0)f'(0)\zeta_{ave} + (\zeta_n - \zeta_m)f(0)[A'_n(0)A_m(0) - A_n(0)A'_m(0)], \end{aligned} \tag{B.5}$$

where $\zeta_{ave} \equiv (\zeta_n + \zeta_m)/2$. The first term on the right-hand side reproduces the Goodmanson [10] result. We have assumed that $f(\zeta)$ is well-enough behaved that surface terms at infinity vanish. One can then evaluate matrix elements over the range $(0, \infty)$ recursively for any combination of products of either even or odd solutions, where simplifications occur since $A'_{n,m}(0) = 0$ or $A_{n,m}(0) = 0$, respectively.

B.2. Recursion relations for oscillator solutions For the ordinary harmonic oscillator, expectation values and matrix elements will be evaluated by integrals of solutions over the range $(-\infty, +\infty)$. But an almost identical derivation to that above allows for the evaluation of related quantities over the half-line $(0, +\infty)$ which will be important for the parity-restricted oscillator (the ‘half’-SHO). For example, if we label $\psi_n(y)$ as a solution to the dimensionless oscillator problem in equation (58), namely

$$\psi_n''(y) = (y^2 - \epsilon_n)\psi_n, \tag{B.6}$$

we can make repeated use of that relation and integrations by part to write

$$J \equiv \int_0^\infty \psi_n(y)\psi_m(y)[f^{(iv)}(y) - 4(y^2 - \epsilon_{ave})f''(y) - 4yf'(y) + (\epsilon_n - \epsilon_m)^2 f(y)] dy, \tag{B.7}$$

in terms of surface terms. In this way, we find that

$$\begin{aligned} J &= -2f'(0)\psi'_n(0)\psi'_m(0) + \psi_n(0)\psi_m(0)[f'''(0) + 2f'(0)\epsilon_{ave}] \\ &\quad f''(0)[\psi'_n(0)\psi_m(0) + \psi_n(0)\psi'_m(0)] - (\epsilon_n - \epsilon_m)f(0)[\psi'_n(0)\psi_m(0) - \psi_n(0)\psi'_m(0)], \end{aligned} \tag{B.8}$$

where $\epsilon_{ave} = (\epsilon_n + \epsilon_m)/2$. Note that for the ‘half’-SHO, only the first term where $\psi'_n(0)$ and $\psi'_m(0)$ are non-zero

We can confirm that this expression encodes the absolute selection rules for matrix elements of the standard oscillator, as in equations (59)–(61). For example, for the dipole matrix elements, we know that for the oscillator only even–odd matrix elements will be relevant, so using $f(y) = y$, we find that

$$J = [(\epsilon_n - \epsilon_m)^2 - 4] \int_0^\infty \psi_n(y)\psi_m(y) dy = 0, \tag{B.9}$$

so that the dipole matrix elements vanish unless $(n - m)^2 = 1$ or $n = m \pm 1$.

Appendix C. Semi-classical probability density for the quantum bouncer

It is straightforward to see how the classical probability distribution in equation (84) for the quantum bouncer arises as the locally averaged limit of the exact quantum mechanical solution. For the bouncer, the solution is given by

$$\psi_n(z) = \sqrt{2}N_n^{(-)} Ai\left(\frac{z}{\rho} - \zeta_n\right), \tag{C.1}$$

where $N_n^{(-)}$ is given by equation (8). Standard handbook [11] results exist for the behavior of $Ai(\zeta)$ and $Ai'(\zeta)$ for large negative values of ζ , namely

$$Ai(-\zeta) \sim \pi^{-1/2}\zeta^{-1/4} \sin\left(\xi + \frac{\pi}{4}\right) \tag{C.2}$$

$$Ai'(-\zeta) \sim \pi^{-1/2}\zeta^{+1/4} \cos\left(\xi + \frac{\pi}{4}\right), \tag{C.3}$$

where $\xi \equiv 2x^{3/2}/3$. The quantum-mechanical probability density is then given by

$$P_{QM}^{(n)}(z) = |\psi_n(z)|^2 = \frac{1}{\rho} \left[\frac{Ai(z/\rho - \zeta_n)}{Ai'(-\zeta_n)} \right]^2 \tag{C.4}$$

$$\sim \frac{\sin^2[2(\zeta_n - z/\rho)^{3/2}/3 + \pi/4]}{\rho\sqrt{\zeta_n(\zeta_n - z/\rho)}}, \tag{C.5}$$

where we use the expression for ζ_n in the large n limit in equation (7) to write

$$\cos\left(\frac{2}{3}\xi + \frac{\pi}{4}\right) \sim \cos\left\{\frac{2}{3}\left(\left[\frac{3\pi}{2}(n - 1/4)\right]^{2/3}\right)^{3/2} + \frac{\pi}{4}\right\} = \cos(n\pi) = \pm 1. \tag{C.6}$$

In the semi-classical limit, the oscillatory component locally averages to 1/2, giving the purely classical result in equation (85). This explicit derivation agrees with the standard result for a purely classical probability distribution for position, namely

$$P_{CL}(x) = \frac{2}{\tau} \sqrt{\frac{m}{2(E - V(x))}}, \tag{C.7}$$

where τ is the classical period, given by

$$\frac{\tau}{2} = \int_a^b \frac{dx}{v(x)} \tag{C.8}$$

with $v(x)$ being the classical speed and a, b are the classical turning points for bounded motion.

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