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Quantum mechanical sum rules for two model systems

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Sum rules have played an important role in the development of many branches of physics since the earliest days of quantum mechanics. We present examples of one-dimensional quantum mechanical sum rules and apply them to the infinite well and the single δ-function potential. These examples illustrate the different ways in which these sum rules can be realized and the varying techniques by which they can be confirmed. We use the same methods to evaluate the second-order energy shifts arising from the introduction of a constant external field, namely the Stark effect.

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I. INTRODUCTION

Quantum mechanical identities that relate time-dependent expectation values, influential in the early days of quantum theory, continue to be useful pedagogical tools. For example, the results often known as Ehrenfest's theorem(s),[1]

$$\langle \hat{p} \rangle_t = m\frac{d\langle x\rangle_t}{dt} \text{ and } m\frac{d^2\langle x\rangle_t}{dt^2} = -\left\langle \frac{dV(x)}{dx} \right\rangle_t, \qquad (1)$$

can be used to show that time-dependent quantum expectation values are related to their corresponding classical equations of motion.[2] Identities restricted to time-independent expectation values evaluated using energy eigenstates, $|n\rangle$, such as the quantum virial theorem

$$\langle n|\hat{T}|n\rangle = \left\langle n \left| \frac{\hat{p}^2}{2m} \right| n \right\rangle = \frac{1}{2}\left\langle n \left| x\frac{dV(x)}{dx} \right| n \right\rangle, \qquad (2)$$

and related hypervirial theorems,[3] are historically and pedagogically valuable because they too have clear classical analogs and can often be evaluated without resorting to direct integration.

Similar relations involving off-diagonal matrix elements, especially sum rules, were also used to dramatic effect in the early days of quantum theory. For example, the Thomas-Reiche-Kuhn energy-weighted sum rule,[4]

$$\sum_k (E_k - E_n)|\langle n|x|k\rangle|^2 = \frac{\hbar^2}{2m}, \qquad (3)$$

was used to describe the physics of electric-dipole interactions with atoms. It was originally obtained by requiring that the Kramers-Heisenberg dispersion relation reduce to the Thomas scattering formula at high energies. The form

$$\sum_k \frac{2m(E_k - E_n)}{\hbar^2}|\langle n|x|k\rangle|^2 = \sum_k f_{n,k} = 1, \qquad (4)$$

was an important experimental check of the oscillator strengths $f_{n,k}$ and a confirmation of the predictions of early quantum theory. Kramer was able to derive this relation in the context of matrix mechanics and reproduced the matrix version of the famous commutation relation $[x,p]=i\hbar$.[5] Other early uses of sum rules included Bethe's study of energy loss mechanisms for charged particles in matter,[6] which made use of the relation

$$\sum_k (E_k - E_n)|\langle n|e^{iqx}|k\rangle|^2 = \frac{\hbar^2 q^2}{2m}, \qquad (5)$$

eventually leading to the Bethe-Bloch formula.

Since then, sum rules have been used in many areas of physics, including atomic,[7] molecular,[8] solid state,[9–12] nuclear,[13–16] and especially particle physics.[17–21] One well-known paper which applied sum rule methods to QCD (Ref. 22) is the tenth most highly cited paper in the particle physics literature and over 2000 papers on QCD sum rules have been published, with 60 appearing in 2007 alone.[23]

The power of such sum rule identities is that they encode a large amount of information about the energy spectrum and energy eigenfunctions of the system in a compact form, often in a way that is amenable to experimental confirmation. These constraints can in turn probe assumptions about the fundamental interactions which were assumed or the methods used to approximate physical systems. For example, QCD sum rules have been used to extract values of both the light and heavy quark masses, which are not otherwise directly measurable quantities.[20]

Despite their historical and contemporary importance, sum rules are not often treated in standard quantum mechanics courses. The Thomas-Reiche-Kuhn sum rule is sometimes included in undergraduate quantum mechanics books,[24] but often only as a problem, and typically only using the harmonic oscillator. This lack of coverage might be due to the paucity of tractable examples in familiar model systems to which students typically are exposed, or the level of mathematical analysis required to verify even the simplest cases.

The purpose of this paper is to provide a suite of one-dimensional sum rules and to demonstrate the techniques required for their confirmation in two model quantum mechanical systems, the infinite well and the single (attractive) δ-function potential. In each case, the sum rules are satisfied in different ways and rely on different evaluation methods (summation techniques and contour integration methods), illustrating the diverse ways in which such sum rules are realized. The level of mathematical detail required is easily accessible to advanced undergraduate students.

Confirming that these sum rues are satisfied is not an empty exercise because it is possible to obtain surprising results, even for simple systems such as the rigid rotator.[25] In addition, energy-weighted sum rule calculations are actually not exotic, because perturbation theory is discussed in standard quantum mechanics textbooks. The second-order shift in the energy due to a perturbation $\tilde{V}(x)$ is given by

$$E_n^{(2)} = \sum_{k\neq n} \frac{|\langle n|\tilde{V}(x)|k\rangle|^2}{(E_n^{(0)} - E_k^{(0)})}, \tag{6}$$

which is the form of an energy-weighted sum rule. By using this connection, we will find that we can use the same techniques for confirming sum rules to evaluate the shift due to the addition of a constant external field, $\tilde{V}(x)=Fx$, namely the Stark shift, in the model systems we consider.

The introduction of sum rules can help students appreciate their use in research applications. It can also help place the methods used in the same context as the more familiar second-order perturbation theory calculations, and show how the related sums over intermediate states can sometimes be done in closed form.

II. SUM RULE EXAMPLES

The derivation of many energy weighted sum rules has been succinctly described as making use of a "…well-known technique which involves closure and evaluating a double commutator in two different ways."[11] Such calculations rely on the fact that the solutions of the system form a complete set of states. For example, consider a system with energy eigenstates satisfying $\hat{H}|n\rangle=E_n|n\rangle$. For an arbitrary operator, $\hat{O}$, we have the sum over off-diagonal matrix elements,

$$\begin{aligned}\sum_{\text{all k}} |\langle n|\hat{O}|k\rangle|^2 &= \sum_{\text{all k}} \langle n|\hat{O}|k\rangle\langle k|\hat{O}|n\rangle \\ &= \langle n|\hat{O}\left\{\sum_{\text{all k}} |k\rangle\langle k|\right\}\hat{O}|n\rangle = \langle n|\hat{O}^2|n\rangle. \end{aligned}\tag{7}$$

The sum over the complete set of intermediate states, $|k\rangle$, may include both an infinite sum (for discrete levels), an integral (for continuum states), or both.

For the special case of $\hat{O}=x$, we obtain the simplest dipole matrix element sum rule given in Bethe and Jackiw,[26,27] namely

$$\sum_k |\langle n|x|k\rangle|^2 = \langle n|x^2|n\rangle \quad (x\text{-closure sum rule}), \tag{8}$$

with an identical sum rule for the off-diagonal matrix elements of the momentum operator.

To derive the Thomas-Reiche-Kuhn sum rule, we start with the commutation relations,

$$[\hat{p},x] = \frac{\hbar}{i} \tag{9a}$$

$$\text{and } [\hat{H},x] = \frac{1}{2m}[\hat{p}^2,x] = \frac{\hbar}{mi}\hat{p}, \tag{9b}$$

where we assumed a standard Hamiltonian of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x). \tag{10}$$

Equation (9a) can be written in the form

$$\frac{\hbar}{i} = \langle n|\hat{p}x - x\hat{p}|n\rangle = \sum_{\text{all k}} [\langle n|\hat{p}|k\rangle\langle k|x|n\rangle - \langle n|x|k\rangle\langle k|\hat{p}|n\rangle], \tag{11}$$

where we have inserted a complete set of states. Equation (9b) can be written as

$$\langle n|\hat{p}|k\rangle = \frac{im}{\hbar}\langle n|[\hat{H},x]|k\rangle = \frac{im(E_n - E_k)}{\hbar}\langle n|x|k\rangle, \tag{12}$$

with a similar expression for $\langle k|\hat{p}|n\rangle$. When used in Eq. (11), Eq. (12) gives the desired result,

$$\frac{\hbar^2}{2m} = \sum_k (E_k - E_n)|\langle n|x|k\rangle|^2. \tag{13}$$

Wang[28] has derived a very general expression for the energy-difference weighted sum rules for the matrix elements of a well-behaved function of x, $F(x)$, namely

$$\sum_k (E_k - E_n)|\langle n|F(x)|k\rangle|^2 = \frac{\hbar^2}{2m}\left\langle n\left|\frac{dF(x)}{dx}\frac{dF^\dagger(x)}{dx}\right|n\right\rangle, \tag{14}$$

which simplifies if the function is Hermitian so that $F(x)=F^\dagger(x)$. This general result can be used to reproduce the Thomas-Reiche-Kuhn sum rule by using $F(x)=x$. We can also derive the Bethe sum rule[6] by using $\hat{O}=e^{iqx}$, in which case we find

$$\sum_k (E_k - E_n)|\langle n|e^{iqx}|k\rangle|^2 = \frac{\hbar^2 q^2}{2m}. \tag{15}$$

If we use $F(x)=x^2$, we obtain the monopole sum rule, which has been used in applications to nuclear collective excitations,[14]

$$\sum_k (E_k - E_n)|\langle n|x^2|k\rangle|^2 = \frac{2\hbar^2}{m}\langle n|x^2|n\rangle. \tag{16}$$

Wang[28] also discussed sum rules involving functions of the momentum operator, and mixed $x,\hat{p}$ relations.

Bethe and Jackiw[26,27] have derived several other sum rules for dipole moment matrix elements by using multiple commutation relations with the Hamiltonian, thus generalizing Eq. (9), and yielding higher powers of the energy difference,

$$\begin{aligned}\sum_k (E_k - E_n)^2|\langle n|x|k\rangle|^2 &= \frac{\hbar^2}{m^2}\langle n|\hat{p}^2|n\rangle \\ &= \frac{2\hbar^2}{m}\{E_n - \langle n|V(x)|n\rangle\},\end{aligned} \tag{17a}$$

$$\sum_k (E_k - E_n)^3|\langle n|x|k\rangle|^2 = \frac{\hbar^4}{2m^2}\left\langle n\left|\frac{d^2V(x)}{dx^2}\right|n\right\rangle, \tag{17b}$$

and

$$\sum_k (E_k - E_n)^4|\langle n|x|k\rangle|^2 = \frac{\hbar^4}{m^2}\left\langle n\left|\left(\frac{dV(x)}{dx}\right)^2\right|n\right\rangle, \tag{17c}$$

where Eqs. (17b) and (17c) are the "force times momentum" and "force squared" sum rules, respectively.

Note that not all of these sum rules are guaranteed to converge,[26] and in our examples, because of the singular nature of the potentials (the infinite well and the single-δ), several of these sum rules will not be applicable.

III. THE INFINITE SQUARE WELL

The infinite square well is the most popular textbook example of a bound state system and is frequently used to introduce students to tractable examples of recent research, such as wave packet revivals.[29] We can confirm many of the sum rules discussed in Sec. II for this case by making use of relatively straightforward techniques to evaluate the infinite sums that appear. (The only example we can find in the literature of the evaluation of sum rules in the context of the infinite well is a short discussion in an appendix of Ref. 14.)

We consider the standard infinite square well defined by

$$V(x)=\begin{cases}0 & (0<x<a)\\ \infty & (x<0 \text{ and } x>a)\end{cases}. \tag{18}$$

The energy eigenstates and corresponding eigenvalues are $\psi_n(x)=\sqrt{2/a}\,\sin(n\pi x/a)$ and $E_n=\hbar^2n^2\pi^2/2ma^2$, where $n=1,2,\ldots$. The expectation value of x^2 required for the closure sum rule in Eq. (8) is easily calculated to be

$$\langle n|x^2|n\rangle = a^2\left(\frac{1}{3}-\frac{1}{2n^2\pi^2}\right). \tag{19}$$

The energy differences needed for the various sum rule calculations are given by

$$E_k-E_n=\frac{\hbar^2\pi^2}{2ma^2}(k^2-n^2), \tag{20}$$

and the off-diagonal matrix elements are given by

$$\langle n|x|k\rangle = \frac{2}{a}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\times\sin\left(\frac{k\pi x}{a}\right)dx \tag{21a}$$

$$=\begin{cases}0 & k+n \text{ even}\\ -(8na/\pi^2)[k/(k^2-n^2)^2] & k+n \text{ odd,}\end{cases} \tag{21b}$$

so that for n even (odd) only odd (even) values of k will contribute. This result is due to the energy eigenfunctions' parity relative to the center of the well at $x=a/2$. For the closure identity in Eq. (8), we need to include the diagonal matrix element,

$$\langle n|x|n\rangle = \frac{a}{2}. \tag{22}$$

This term does not contribute to the other sum rules, because the $k=n$ term is suppressed by the (E_k-E_n) energy difference factor. In contrast to potential energy functions that are symmetric about the origin, such as the harmonic oscillator potential and the single δ-function potential, the standard infinite square well potential as defined in Eq. (18) is not symmetric, and we must consider the $k=n$ case for the closure identity.

The position closure sum rule in Eq. (8) reads

$$\sum_{\text{all } k}|\langle n|x|k\rangle|^2=\left(\frac{a}{2}\right)^2+\left(\frac{8na}{\pi^2}\right)^2\sum_k\frac{k^2}{(k^2-n^2)^4}, \tag{23}$$

where the sum is over even (odd) values of k if n is odd (even). Equation (23) is the first of many examples that we will encounter where we require infinite sums of the form

$$S_p^{(\pm)}(z)=\sum_k\frac{1}{(k^2-z^2)^p}, \tag{24}$$

where z takes on integer values and the sum is over odd, $S^{(-)}$, or even, $S^{(+)}$, values of k. For example, the sum in Eq. (23) can be written in the form

$$\sum_k\frac{k^2}{(k^2-n^2)^4}=\sum_k\frac{(k^2-n^2+n^2)}{(k^2-n^2)^4}=S_3^{(\pm)}(n)+n^2S_4^{(\pm)}(n). \tag{25}$$

We evaluate all of the sums required in this section using standard series expansions in Appendix A. However, current computer algebra systems such as MATHEMATICA can easily handle such sums. Students may be allowed on the first pass to use such tools and then asked to delve more deeply into the methods used to obtain the general mathematical results for this class of problems.

For example, in modified MATHEMATICA syntax, the sum over even integers k (relevant for n odd), yields

```
Sum[k^2/(k^2-z^2)^4,{k,2,Infinity,2}]
=(-12 Pi Cot[Pi z/2]-6 Pi^2 z Csc[Pi z/2]^2
+2 Pi^4 z^3 Cot[Pi z/2]^2 Csc[Pi z/2]^2
+Pi^4 z^3  Csc[Pi z/2]^4)/768z^5
```

so that for odd integer values of $z=n$, we have (by hand or by using Assuming−>$z\in$ Integers in MATHEMATICA)

$$\sum_{k\text{ even}}\frac{k^2}{(k^2-n^2)^4}=\frac{\pi^4n^3-6\pi^2n}{768n^5}=\frac{\pi^4}{768n^2}-\frac{\pi^2}{128n^4}. \tag{26}$$

We obtain the same function of n for the sum over odd values of k (relevant for even n). A trivial modification of the MATHEMATICA code is all that is required. If we use this result in Eq. (23), we find that

$$\sum_{\text{all } k}|\langle n|x|k\rangle|^2=|\langle n|x|n\rangle|^2+\sum_{k\neq n}|\langle n|x|k\rangle|^2 \tag{27a}$$

$$=\frac{a^2}{4}+\frac{64a^2n^2}{\pi^4}\left(\frac{\pi^4}{768n^2}-\frac{\pi^2}{128n^4}\right) \tag{27b}$$

$$=a^2\left(\frac{1}{3}-\frac{1}{2n^2\pi^2}\right)=\langle n|x^2|n\rangle, \tag{27c}$$

as expected.

The Thomas-Reiche-Kuhn sum rule is then given by

$$\sum_k(E_k-E_n)|\langle n|x|k\rangle|^2=\left(\frac{\hbar^2}{2m}\right)\left(\frac{64n^2}{\pi^2}\right)\sum_k\frac{k^2}{(k^2-n^2)^3}, \tag{28}$$

where the sum over k is only for even (odd) values for n odd (even). These sums can also be done in closed form, and we find

$$I_n^{(+)}(z) \equiv \sum_{k \text{ even}} \frac{k^2}{(k^2-z^2)^3} = S_2^{(+)}(z) + z^2 S_3^{(+)}(z) \tag{29a}$$

$$= \frac{1}{64z^3}\left[\pi^2 z \csc^2\left(\frac{\pi z}{2}\right) + 2\pi \cot\left(\frac{\pi z}{2}\right) - \pi^3 z^2 \cot\left(\frac{\pi z}{2}\right)\cos^2\left(\frac{\pi z}{2}\right)\right], \tag{29b}$$

$$I_n^{(-)}(z) \equiv \sum_{k \text{ odd}} \frac{k^2}{(k^2-z^2)^3} = S_2^{(-)}(z) + z^2 S_3^{(-)}(z) \tag{29c}$$

$$= \frac{1}{64z^3}\left[\pi^2 z \sec^2\left(\frac{\pi z}{2}\right) - 2\pi \tan\left(\frac{\pi z}{2}\right) + \pi^3 z^2 \tan\left(\frac{\pi z}{2}\right)\sec^2\left(\frac{\pi z}{2}\right)\right]. \tag{29d}$$

Note the similarities in form. If we substitute the appropriate odd and even values of n in each case, we find that

$$I_n^{(+)}(n) = I_n^{(-)}(n) = \frac{\pi^2}{64n^2}, \tag{30}$$

for all integer values of n. This result, when substituted into Eq. (28), directly confirms the Thomas-Reiche-Kuhn sum rule.

The verification of the monopole sum rule in Eq. (16) requires a small, but important, modification of the summation methods. The off-diagonal matrix elements required for $k \neq n$ are

$$\langle n|x^2|k\rangle = \frac{(-1)^{k-n} 8a^2 n}{\pi^2}\left(\frac{k}{(k^2-n^2)^2}\right). \tag{31}$$

For $k=n$ we use the result in Eq. (19). Because the $k=n$ term does not contribute to the sum (because of the associated energy difference factor), the left-hand side of Eq. (16) reduces to

$$\sum_k (E_k - E_n)|\langle n|x^2|k\rangle|^2 = \left(\frac{\hbar^2\pi^2}{2ma^2}\right) \times \left(\frac{64n^2a^4}{\pi^4}\right)\sum_{k\neq n} \frac{k^2}{(k^2-n^2)^3}, \tag{32}$$

and we must sum over all values of $k \neq n$ because the even/odd pattern in the dipole matrix elements is not present in this case.

To evaluate this sum we first generalize the sum to noninteger values of n (see Appendix A) and rewrite the sum as

$$T(z;n) \equiv \sum_{k\neq n} \frac{k^2}{(k^2-z^2)^3} = \left[\sum_{\text{all } k} \frac{k^2}{(k^2-z^2)^3}\right] - \frac{n^2}{(n^2-z^2)^3}. \tag{33}$$

The second term corresponds to the "missing" term in the $k \neq n$ sum. The first sum can be evaluated for arbitrary z, giving

$$T(z;n) = \left(\frac{\pi \cot(\pi z) + \pi^2 z \csc^2(\pi z) - 2\pi^3 z^2 \cot(\pi z)\csc^2(\pi z)}{16z^3}\right) - \frac{n^2}{(n^2-z^2)^3}. \tag{34}$$

Because we will take the limit $z \to n$, we write $z = n + \epsilon$ for general n and find that both terms on the right-hand side of Eq. (34) have factors that diverge as $1/\epsilon^3$, $1/\epsilon^2$, and $1/\epsilon$. If we expand both terms in small values of ϵ, we find that these divergences cancel, leaving the finite result

$$\lim_{z\to n} T(z;n) = \lim_{\epsilon\to 0} T(n+\epsilon;n) = T(n) = \frac{\pi^2}{16n^2}\left(\frac{1}{3} - \frac{1}{2n^2\pi^2}\right), \tag{35}$$

which when inserted into Eq. (32) reproduces the right-hand side of Eq. (16).

Many of the other sum rules discussed in Sec. II, such as those that require derivatives of the potential energy function, Eqs. (17b) and (17c), are not well-defined for the infinite square well (or the single δ-function in Sec. IV) due to the singular nature of the potential energy function. Although the matrix elements $\langle n|e^{iqx}|k\rangle$ required for the Bethe sum rule in Eq. (5) are easily obtained in closed form, the summation methods discussed here are not immediately applicable.

We can now use identical methods to evaluate the second-order shift of the energy levels of the infinite square well with the addition of a linear potential, $V'(x) = Fx$, namely the Stark effect. In our choice of geometry the infinite square well potential is not symmetric, and the first-order energy shift is nonvanishing and is given by

$$E_n^{(1)} = \langle n|Fx|n\rangle = \frac{aF}{2}. \tag{36}$$

The second-order shift has been evaluated by Mavromatis for the ground state[30] and extended to a general state[31,32] by using variations on the Dalgarno-Lewis method.[33] If we explicitly write the standard expression for the second-order energy shift, we have

$$E_n^{(2)} = \sum_{k\neq n} \frac{|\langle n|Fx|k\rangle|^2}{(E_n^{(0)} - E_k^{(0)})} = -\left(\frac{F^2 2ma^2}{\hbar^2}\right) \times \left(\frac{8na}{\pi^2}\right)^2 \sum_k \frac{k^2}{(k^2-n^2)^5}, \tag{37}$$

which is formally identical to the type of summations discussed here. By using either MATHEMATICA or the results of Appendix A, we find that the sum (for n even or odd) is given by

$$\sum_k \frac{k^2}{(k^2-n^2)^5} = \frac{15\pi^2 n - \pi^4 n^3}{3072 n^7}, \tag{38}$$

so that

$$E_n^{(2)} = -F^2\left(\frac{ma^4}{\hbar^2}\right)\left(\frac{15 - (n\pi)^2}{24\pi^2 n^4}\right). \tag{39}$$

The overall n-dependent form agrees with the results of Mavromatis,[30–32] who considered the symmetric infinite well for which the first-order correction vanishes. Equation (39) is interesting in itself because the second-order shift for the ground state is negative [as it must be, because all states contributing to Eq. (37) are higher in energy], but for $n=2$ and higher, the shift changes sign. This change of sign is in contrast to the behavior of the harmonic oscillator, where the second-order shift is always negative, independent of quantum number.

IV. THE SINGLE δ-FUNCTION POTENTIAL

Another popular model system in which to investigate sum rule and perturbation theory results is the single (attractive) δ-function potential defined by

$$V_\delta(x) = -g\,\delta(x). \tag{40}$$

The use of δ-function potentials as soluble models of potential barriers or wells has a long history in quantum mechanics, going back at least to Kronig and Penney,[34] who considered a series of equidistant rectangular barriers and then took the limit where the width of these barriers is made infinitely small and their height V_0 infinitely large, while not using the δ-function notation.

Morse and Feshbach[35] explicitly considered the form in Eq. (40), and used the correct (dis)continuity condition on the energy eigenfunction at the origin,

$$\psi'(0^+) - \psi'(0^-) = -\frac{2mg}{\hbar^2}\psi(0). \tag{41}$$

They cited this model as being useful in the study of nuclear forces and discussed the single bound state as well as scattering solutions. Frost[36] considered single and multiple attractive δ-function potentials as models of hydrogenlike atoms, the hydrogen moleculeion, and more complex systems. He was perhaps the first to explicitly comment on the similarities of the energy eigenvalue and eigenfunction for the single bound state of this system to the ground state of the Coulomb problem. Since then, single and multiple δ-function potentials have been widely used in model calculations in the pedagogical and research literature.[37]

Compared to the two other most widely used simple 1D models, the infinite well and harmonic oscillator, the δ-function potential has the advantage that it has both bound and continuum solutions, as does the Coulomb potential, and so it presents new features compared to purely discrete spectra.

The single bound ($E<0$) state for the potential in Eq. (40) is given by

$$\psi_0(x) = \sqrt{K_0}e^{-K_0|x|}, \tag{42}$$

where $K_0 = mg/\hbar^2$. The corresponding bound state energy eigenvalue is

$$E_0 = -\frac{mg^2}{2\hbar^2} = -\frac{\hbar^2 K_0^2}{2m}. \tag{43}$$

Comparisons to the ground state of the hydrogen atom can be made if we write the Coulomb potential as $V_c(r) = -g/r$ and let $a_0 = 1/K_0$ in Eqs. (42) and (43). Not only does the form of the ground-state energy in Eq. (43) match that of the Coulomb potential, but the form of the energy eigenfunction in Eq. (42) does as well.

For use in confirming the closure relations in Eq. (8), we find that for the ground-state energy eigenfunction

$$\langle 0|x^2|0\rangle = \frac{1}{2K_0^2}. \tag{44}$$

The $E>0$ continuum states can be classified by their parity and are given by

$$\psi_k^{(-)}(x) = \frac{1}{\sqrt{\pi}}\sin(kx) \tag{45a}$$

$$\psi_k^{(+)}(x) = \frac{1}{\sqrt{\pi(k^2+K_0^2)}}(K_0\sin(k|x|) - k\cos(kx)), \tag{45b}$$

both of which have the same free-particle energy $E_k = \hbar^2k^2/2m$. The combination of the single bound state in Eq. (42) and the continuum states in Eq. (45) has been shown to form a complete set of states.[38] The effect of the continuum states on a simple perturbation theory calculation has also been demonstrated by Kiang.[39]

We will consider here only the $|n\rangle = |0\rangle$ case for the various sum rules, as the others using purely continuum states do not converge. Because of the symmetry of the system, parity arguments dictate that the only nonzero dipole matrix elements connecting the single ground state to the continuum will arise from the $\psi_k^{(-)}(x)$ states. We find that

$$\langle 0|x|k^{(-)}\rangle = \int_{-\infty}^{+\infty}(\sqrt{K_0}e^{-K_0|x|})x\left(\frac{1}{\sqrt{\pi}}\sin(kx)\right)dx = 4\sqrt{\frac{K_0^3}{\pi}}\frac{k}{(K_0^2+k^2)^2}. \tag{46}$$

The energy differences are given by

$$E_k - E_0 = \frac{\hbar^2}{2m}(k^2+K_0^2), \tag{47}$$

and we note the similarities in form between these two expressions and the corresponding results for the infinite square well in Eqs. (20) and (21b).

The dipole matrix element closure relation in Eq. (8) becomes

$$\sum_k |\langle 0|x|k^{(-)}\rangle|^2 = \left(\frac{16K_0^3}{\pi}\right)\int_0^\infty \frac{k^2}{(k^2+K_0^2)^4}dk = \frac{1}{2K_0^2} = \langle 0|x^2|0\rangle. \tag{48}$$

The integral can be done by standard methods, and agrees with the value in Eq. (44).

The left-hand side of the Thomas-Reiche-Kuhn sum rule in Eq. (3) gives

$$\int_0^\infty (E_k - E_0)|\langle 0|x|k^{(-)}\rangle|^2 dk = \frac{\hbar^2}{2m}\left(\frac{16K_0^3}{\pi}\right)\int_0^{+\infty}\frac{k^2}{(k^2+K_0^2)^3}dk = \frac{\hbar^2}{2m}, \tag{49}$$

as expected. Note the similarity in form of these integral expressions to the summation results for the infinite well in Eqs. (28) and (23).

To confirm the monopole sum rule in Eq. (16), we require the off-diagonal matrix elements of x^2 for which only the even continuum states in Eq. (45b) contribute, giving

$$\langle 0|x^2|k^{(+)}\rangle = 8\sqrt{\frac{K_0^3}{\pi(k^2+K_0^2)}}\frac{k}{(k^2+K_0^2)^2}. \tag{50}$$

We find that

$$\sum_k (E_k - E_0)|\langle 0|x^2|k^{(+)}\rangle|^2 = \left(\frac{\hbar^2}{2m}\right)\left(\frac{64K_0^3}{\pi}\right)\int_0^\infty \frac{k^2}{(k^2+K_0^2)^4}dk = \frac{\hbar^2}{mK_0^2}. \tag{51}$$

Note that factors of $(k^2+K_0^2)$ from the energy difference and the energy eigenfunction normalization in the numerator and denominator, respectively, cancel.

The Stark effect for the single δ-function potential has been analyzed using exact results for the Airy function solutions,[40,41] as well as the Dalgarno-Lewis method.[42] If we use the dipole matrix elements in Eq. (46), we can evaluate the second-order energy shift directly, using the same kinds of straightforward integrals encountered so far. We find that

$$E_0^{(2)} = \int_k \frac{|\langle 0|Fx|k^{(-)}\rangle|^2}{(E_0^{(0)} - E_k^{(0)})} \tag{52a}$$

$$= -\frac{2mF^2}{\hbar^2}\left(\frac{16K_0^3}{\pi}\right)\int_0^\infty \left\{\frac{1}{(k^2+K_0^2)}\right\}\frac{k^2}{(k^2+K_0^2)^4}dk, \tag{52b}$$

which agrees with the results of Refs. 40–42, when put into this notation. We note that the entire contribution of the Stark shift to the ground-state energy in this case comes from the continuum states. This result is one of the few examples of the explicit evaluation of the contribution of the continuum terms.

We recall that, for the hydrogen atom ground state, the total second-order shift can be written in the form[43]

$$E_0^{(2)}(\text{H-atom}) = -\frac{9}{4}\left(\frac{F^2 a_0^3}{g}\right). \tag{53}$$

This result comes from summing the contributions of both the bound states and continuum states. Ruffa has evaluated the continuum contribution to Eq. (53) in terms of a single integral and found a net contribution of 0.4184 to the total $9/4=2.25$ value of the prefactor.[44] We compare the second-order Stark result in Eq. (52b), namely $5/8=0.625$, to that partial contribution, and note that the continuum plays a slightly more important role in the single delta function case because there is only one bound state.

The Bethe sum rule is given by

$$B = \sum_k (E_k - E_0)|\langle 0|e^{iqx}|k\rangle|^2 = \frac{\hbar^2 q^2}{2m}. \tag{54}$$

In this case there are two contributions to the left-hand side coming from the even (e) or odd (o) continuum states, namely

$$B = B_e + B_o = \int_0^\infty (E_k - E_0)|\langle 0|\cos(qx)|k^{(+)}\rangle|^2 dk \tag{55a}$$

$$+ \int_0^\infty (E_k - E_0)|\langle 0|\sin(qx)|k^{(-)}\rangle|^2 dk. \tag{55b}$$

We consider each term separately. The first matrix element of interest is

$$I_o = \langle 0|\sin(qx)|k^{(-)}\rangle = \sqrt{\frac{4K_0}{\pi}}\int_0^\infty e^{-K_0 x}\sin(qx)\sin(kx)dx \tag{56a}$$

$$= \sqrt{\frac{4K_0}{\pi}}\left[\frac{2kqK_0}{[(k+q)^2+K_0^2][(k-q)^2+K_0^2]}\right], \tag{56b}$$

where we have used the symmetry of the energy eigenfunctions to evaluate the integral over positive values of x only. Because $E_k - E_0 = \hbar^2(k^2+K_0^2)/2m$, we find

$$B_o = \frac{\hbar^2 q^2}{2m}\left(\frac{16K_0^3}{\pi}\right)\int_0^\infty \frac{k^2(k^2+K_0^2)}{[(k+q)^2+K_0^2]^2[(k-q)^2+K_0^2]^2}dk. \tag{57}$$

The use of an integrated mathematics package returns the correct value for the integral if we correctly interpret the many cautionary restrictions on the values of K_0 and q. However, given the complicated nature of the intermediate results coming from such programs, it is important to be able to check the expressions by hand. In this case the evaluation involves extending the integral over the entire real line (because the integrand is an even function of k) and then using contour integration methods (see Appendix B for details). The result is

$$B_o = \left(\frac{\hbar^2 q^2}{2m}\right)\left[\frac{K_0^2 + q^2/2}{K_0^2+q^2}\right]. \tag{58}$$

For the even case we require the matrix element

$$I_e = \langle 0|\cos(qx)|k^{(+)}\rangle = \sqrt{\frac{4K_0}{\pi(K_0^2+k^2)}}\int_0^\infty e^{-K_0 x}\cos(qx) \times [K_0\sin(kx) - k\cos(kx)]dx \tag{59a}$$

$$= \sqrt{\frac{4K_0}{\pi(K_0^2+k^2)}}\left[\frac{-2kK_0q^2}{[(k+q)^2+K_0^2][(k-q)^2+K_0^2]}\right]. \tag{59b}$$

The even contribution to the sum rule becomes

$$B_{\mathrm{e}} = \int_0^{\infty} (E_k - E_0)|\langle 0|\cos(qx)|k^{(+)}\rangle|^2 dk \tag{60a}$$

$$= \left(\frac{\hbar^2 q^2}{2m}\right) \times \left(\frac{8K_0^3 q^2}{\pi}\right) \int_{-\infty}^{+\infty} \frac{k^2}{[(k+q)^2 + K_0^2]^2[(k-q)^2 + K_0^2]^2} dk. \tag{60b}$$

The integral can again be done with similar contour methods, giving the result

$$B_{\mathrm{e}} = \left(\frac{\hbar^2 q^2}{2m}\right)\left\{\frac{q^2/2}{K_0^2 + q^2}\right\}, \tag{61}$$

which can be combined with Eq. (58) to give

$$B = B_{\mathrm{o}} + B_{\mathrm{e}} = \frac{\hbar^2 q^2}{2m}, \tag{62}$$

as expected.

V. CONCLUSIONS AND DISCUSSION

We have presented an array of familiar and not so familiar one-dimensional sum rules, several of which have been useful in the development of many fields of physics. By using two standard model systems as testbeds, we have illustrated the diverse ways in which such sum rules are confirmed, emphasizing the different techniques (infinite summation tricks and contour integration methods). Although the evaluation of the necessary sums and integrals can be simplified by the use of software, we have provided the details necessary to demonstrate the same results.

We have also noted the similarities of some of the expressions that arise for the same sum rules in the infinite square well and single δ-potential cases. Despite the qualitatively different physical behavior of the two systems, they both begin with free-particle solutions. The connections between these two model systems are seldom stressed, but appear very natural in the sum rule calculations.

APPENDIX A: INFINITE SUMS FOR THE SQUARE WELL PROBLEM

Many of the sum rule and second-order perturbation theory results in Sec. III for the infinite square well involve the evaluation of infinite sums of the form

$$S_p^{(+)}(z) = \sum_{\text{even } k} \frac{1}{(k^2 - z^2)^p} \tag{A1}$$

and

$$S_p^{(-)}(z) = \sum_{\text{odd } k} \frac{1}{(k^2 - z^2)^p}. \tag{A2}$$

Both expressions are eventually evaluated using integer values of $z=n$, with n odd and even, respectively, so no divergences occur. Although software can evaluate such sums, it is important for some students and many instructors to be able to derive them from scratch. To that end we provide a brief, but self-contained and complete review of the mathematical tools necessary for their derivation.

We begin by considering the general expression

$$S_p(z) \equiv \sum_{k=1}^{\infty} \frac{1}{(k^2 - z^2)^p}, \tag{A3}$$

where the sum is over all positive integer values of k. The basic result we require is for $p=1$, namely

$$S_1(z) = \sum_{k=1}^{\infty} \frac{1}{(k^2 - z^2)} = \frac{1}{2z^2} - \frac{\pi\cot(\pi z)}{2z}, \tag{A4}$$

which appears, for example, in Ref. 45. This standard result can be derived at a more fundamental level from a Fourier series expansion[46] by evaluating the Fourier components of the expansion

$$\cos(zx) = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos(nx) + b_n \sin(nx)], \tag{A5}$$

over the interval $(-\pi, +\pi)$; note that here z is considered a constant. The Fourier coefficients can be evaluated using standard integrals, and we obtain

$$\cos(zx) = \frac{\sin(z\pi)}{z\pi} - \sum_{n=1}^{\infty}\left[\frac{2z\sin(\pi z)\cos(n\pi)}{\pi(n^2 - z^2)}\right]\cos(nx), \tag{A6}$$

because $b_n=0$ by symmetry. If we specialize to $x=\pi$ and use the fact that $\cos^2(n\pi)=1$, we find

$$\pi\cot(\pi z) = \frac{1}{z} - 2z\sum_{n=1}^{\infty}\frac{1}{(n^2 - z^2)}. \tag{A7}$$

We note that this partial fraction expansion of $\cot(\pi z)$ correctly encodes the information on the divergences of the function at all integer (positive, negative, and zero) values of z. We rewrite Eq. (A7) and find that

$$S_1(z) = \sum_{n=1}^{\infty}\frac{1}{(n^2 - z^2)} = \frac{1}{2z}\left(\frac{1}{z} - \pi\cot(\pi z)\right) = \frac{1}{2z^2} - \frac{\pi\cot(\pi z)}{2z}, \tag{A8}$$

confirming Eq. (A4). Such sums are useful in that they can be used to evaluate quantities such as the Riemann zeta function, defined by

$$\zeta(s) \equiv \sum_{n=1}^{\infty}\frac{1}{n^s}, \tag{A9}$$

giving

$$\zeta(2) = S_1(z=0) = \sum_{n=1}^{\infty}\frac{1}{n^2} = \frac{\pi^2}{6}, \tag{A10}$$

as the $z\to 0$ limit of Eq. (A8). (Such results can be directly related to integrals that appear frequently in the evaluation of quantities related to blackbody radiation[47] and can therefore be reinforced through such examples.)

If we differentiate the result in Eq. (A8) with respect to z, we find that

$$\frac{d}{dz}S_1(z) = 2z\sum_{k=1}^{\infty}\frac{1}{(k^2-z^2)^2} = 2zS_2(z), \tag{A11}$$

so that in general

$$S_{p+1}(z) = \frac{1}{2z}\frac{dS_p(z)}{dz}, \tag{A12}$$

thereby generating sums of arbitrarily high power. For example, Eq. (A12) gives

$$S_2(z) = \frac{\csc^2(\pi z)[-2+2\pi^2z^2+2\cos(2\pi z)+\pi z\sin(2\pi z)]}{8z^4}, \tag{A13}$$

which implies that $\zeta(4)=S_2(z=0)=\pi^4/90$.

Because our interest is often in sums restricted to even or odd integers, we write

$$S_1(z) = \sum_{k=1}^{\infty}\frac{1}{(k^2-z^2)} = \sum_{k\ \mathrm{even}}^{\infty}\frac{1}{(k^2-z^2)} + \sum_{k\ \mathrm{odd}}^{\infty}\frac{1}{(k^2-z^2)}$$
$$\equiv S_1^{(+)}(z) + S_1^{(-)}(z). \tag{A14}$$

We note that

$$S_1^{(+)}(z) = \sum_{k\ \mathrm{even}}^{\infty}\frac{1}{(k^2-z^2)} = \sum_{l=1}^{\infty}\frac{1}{((2l)^2-z^2)} \tag{A15a}$$

$$= \frac{1}{4}\sum_{l=1}^{\infty}\frac{1}{(l^2-(z/2)^2)} = \frac{1}{4}S_1\left(\frac{z}{2}\right) \tag{A15b}$$

$$= \frac{1}{2z^2} - \frac{\pi\cot(\pi z/2)}{4z}, \tag{A15c}$$

which gives

$$S_1^{(-)}(z) = S_1(z) - S_1^{(+)}(z) = \frac{\pi}{4z}\left[\cot\left(\frac{\pi z}{2}\right) - 2\cot(\pi z)\right]$$
$$= \frac{\pi\tan(\pi z/2)}{4z}, \tag{A16}$$

where we have used half-angle formulas in the last step. The expressions in Eqs. (A15c) and (A16) can be confirmed using MATHEMATICA.

The sums over higher powers of even/odd values of n require us to evaluate $S_p^{(+)}(x)$ and $S_p^{(-)}(x)$ in Eq. (A2), obtained by repeated use of the differentiation trick in Eq. (A12). For example, we can obtain results such as

$$S_2^{(+)}(z) = \frac{\csc^2(\pi z/2)[-4+\pi^2z^2+4\cos(\pi z)+\pi z\sin(\pi z)]}{16x^4} \tag{A17a}$$

and

$$S_2^{(-)}(z) = \frac{\pi\sec^2(\pi z/2)[\pi z-\sin(\pi z)]}{16z^3}. \tag{A17b}$$

APPENDIX B: CONTOUR INTEGRALS

The explicit evaluation of the integrals in Eqs. (57) and (60b) by contour integration can be done by extending the region of integration over the entire real axis. A contour consisting of a semicircle of radius R can then be used because the integrands both have simple (double) poles at $z_0^{(\pm)} = \pm q + iK_0$ in the upper-half plane. The contribution to the contour integral over the circular arc vanishes as $R\to\infty$, leaving

$$\int_{-\infty}^{+\infty}F(k)dk = 2\pi i\sum_i R_i, \tag{B1}$$

where the residues are given by

$$R_i = \frac{1}{(n-1)!}\left[\left(\frac{d}{dz}\right)^{n-1}[(z-z_0^{(i)})^nF(z)]\right]_{z\to z_0^{(i)}}, \tag{B2}$$

for $z_0^{(i)}=z_0^{(\pm)}$ and where $n=2$ in this case.

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