Quantum-Mechanical Sum Rules

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Sum rules are derived for expressions of the form $\sum_k \omega_{kn}{}^a |A_{kn}|^2$; $|a|=0,1,\cdots$. Application of the sum rules are given for various forms of A.

I. INTRODUCTION

In estimating intensity of radiation, and in other applications, it is useful to consider sums of electric-dipole-moment matrix elements, weighted by a power of the frequency

$$X_n{}^a=\sum_k \omega_{kn}{}^a |x_{kn}|^2. \tag{1}$$

Here x_{kn} is evaluated between energy eigenstates k and n, n being a discrete, normalizable state; ω_{kn} is the frequency of these two states: $\omega_{kn}=(E_k-E_n)/\hbar$; a is a non-negative integer; and the sum in k extends over all energy eigenstates. By defining

$$|\mathbf{r}_{kn}|^2=\mathbf{r}_{kn}\cdot\mathbf{r}_{nk}=|x_{kn}|^2+|y_{kn}|^2+|z_{kn}|^2,$$

a symmetric expression may be given

$$R_n{}^a=\tfrac{1}{3}\sum_k \omega_{kn}{}^a |\mathbf{r}_{kn}|^2. \tag{2}$$

Sum rules which give a closed expression for $R_n{}^a$ are well known for $a=0$, 1, 2, 3, 4.[1] These are

$$\begin{aligned}
&R_n{}^0=\tfrac{1}{3}\langle n|r^2|n\rangle,\\
&R_n{}^1=\hbar/2m,\\
&R_n{}^2=(1/3m^2)\langle n|p^2|n\rangle=(2/3m)\langle n|E_n-V|n\rangle,\\
&R_n{}^3=(\hbar/6m^2)\langle n|\nabla^2 V|n\rangle,\\
&R_n{}^4=(1/3m^2)\langle n|(\boldsymbol{\nabla} V)^2|n\rangle.
\end{aligned} \tag{3}$$

In the above, V is the potential occurring in the Hamiltonian, which is assumed to have the simple form

$$\begin{aligned}
H&=(p^2/2m)+V(r),\\
H|n\rangle&=E_n|n\rangle.
\end{aligned} \tag{4}$$

The $a=1$ case is the famous Thomas-Reiche-Kuhn *oscillator-strength sum rule,* which was important in the development of quantum mechanics. The usual derivation[1] of the results given in (3) proceeds by exploiting the commutation relations between $\mathbf{r}$ and $\mathbf{p}$ and using the identity

$$\langle k|\mathbf{p}|n\rangle=im\omega_{kn}\langle k|\mathbf{r}|n\rangle. \tag{5}$$

In the present paper using a systematic technique which differs from the usual derivation we give general sum rules, valid when a is any non-negative integer, and x is replaced by any operator.

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[1] H. A. Bethe, *Intermediate Quantum Mechanics* (W. A. Benjamin, Inc., New York, 1964).

II. DERIVATION OF GENERAL SUM RULES

To derive the desired result, we investigate a general sum rule of the form

$$S_n{}^a=\sum_k (E_k-E_n)^a|A_{kn}|^2=\sum_k (E_k-E_n)^a A_{kn}A^\dagger{}_{nk}, \tag{6}$$

where A is any operator. The states k, n are eigenstates of a Hamiltonian, which we take to be arbitrary, i.e., not necessarily of the simple form (4). The state n is assumed to be normalizable.[2]

Consider the quantity

$$e^{itH/\hbar}Ae^{-itH/\hbar}, \tag{7a}$$

which is equal to the series

$$e^{itH/\hbar}Ae^{-itH/\hbar}=\sum_{a=0}^{\infty}\left(\frac{it}{\hbar}\right)^a\frac{A_a}{a!}, \tag{7b}$$

where the commutant A_a is defined recursively by

$$\begin{aligned}
A_0&=A,\\
A_a&=[H,A_{a-1}].
\end{aligned} \tag{7c}$$

Next consider

$$\langle n|A^\dagger e^{itH/\hbar}Ae^{-itH/\hbar}|n\rangle. \tag{8a}$$

Inserting a complete set of energy eigenstates, (8a) becomes

$$\begin{aligned}
\langle n|A^\dagger e^{itH/\hbar}Ae^{-itH/\hbar}|n\rangle
&=\sum_k \langle n|A^\dagger e^{itH/\hbar}|k\rangle\langle k|Ae^{-itH/\hbar}|n\rangle\\
&=\sum_k e^{it\omega_{kn}}A_{kn}A^\dagger{}_{nk}.
\end{aligned} \tag{8b}$$

Expanding the exponential, and interchanging the orders of summation, yields

$$\langle n|A^\dagger e^{itH/\hbar}Ae^{-itH/\hbar}|n\rangle
=\sum_a \frac{(it)^a}{a!}\sum_k \omega_{kn}{}^a|A_{kn}|^2=\sum_a\left(\frac{it}{\hbar}\right)^a\frac{S_n{}^a}{a!}. \tag{8c}$$

On the other hand, we can use formula (7b) to expand (8a).

$$\langle n|A^\dagger e^{itH/\hbar}Ae^{-itH/\hbar}|n\rangle=\sum_a\left(\frac{it}{\hbar}\right)^a\frac{1}{a!}\langle n|A^\dagger A_a|n\rangle. \tag{9}$$

[2] It is evident that the considerations in this paper may be extended trivially to give sum rules for expressions of the form $\sum_k(\lambda_k-\lambda_n)^a|A_{kn}|^2$, where λ_k is the eigenvalue of a Hermitian operator L, which possesses a complete set of eigenstates; the states k, n are eigenstates of this operator, with n a normalizable state; and the summation extends over the complete set of eigenstates.

Comparing (9) with (8c) gives the preliminary sum rule

$$S_n^a = \langle n|A^\dagger A_a|n\rangle. \quad (10)$$

Equation (10) in principle gives a closed expression for S_n^a. One needs to commute A with H a times to get A_a and then evaluate $\langle n|A^\dagger A_a|n\rangle$. However (10) can be simplified by making use of the relation

$$\langle n|A^\dagger A_a|n\rangle = \langle n|A_b{}^\dagger A_{a-b}|n\rangle, \quad a \geqslant b \quad (11a)$$

To prove (11a), we note that by definition of A_a

$$\langle n|A^\dagger A_a|n\rangle = \langle n|A^\dagger H A_{a-1} - A^\dagger A_{a-1}H|n\rangle. \quad (11b)$$

Since $|n\rangle$ is an energy eigenstate, the second term on the right of (11b) gives

$$\langle n|A^\dagger A_{a-1}H|n\rangle = E_n\langle n|A^\dagger A_{a-1}|n\rangle = \langle n|HA^\dagger A_{a-1}|n\rangle. \quad (11c)$$

Hence we have

$$\begin{aligned}\langle n|A^\dagger A_a|n\rangle &= \langle n|[A^\dagger H - HA^\dagger]A_{a-1}|n\rangle \\ &= \langle n|[H,A]^\dagger A_{a-1}|n\rangle \\ &= \langle n|A_1{}^\dagger A_{a-1}|n\rangle. \end{aligned} \quad (11d)$$

Evidently this procedure may be continued b times to yield (11a). Thus we can give many, formally different, expressions for each S_n^a

$$\begin{aligned} S_n^a &= \langle n|A^\dagger A_a|n\rangle = \langle n|A^\dagger A_{a-1}|n\rangle = \cdots \\ &= \langle n|A_{a-1}{}^\dagger A_1|n\rangle = \langle n|A_a{}^\dagger A|n\rangle. \end{aligned} \quad (12a)$$

Linear combination between these can give still more, formally different, sum rules. For practical purposes, the simplest expression for S_n^a is the one for which A needs to be commuted with H the least number of times, since in general the A_a's increase in complexity with increasing a. Thus the sum rules we shall be concerned with for the most part are

$$\begin{aligned} S_n^{2a} &= \langle n|A_a{}^\dagger A_a|n\rangle, \\ S_n^{2a+1} &= \langle n|A_a{}^\dagger A_{a+1}|n\rangle = \langle n|A_{a+2}{}^\dagger A_a|n\rangle \\ &= \tfrac{1}{2}\langle n|A_a{}^\dagger A_{a+1} + A_{a+1}{}^\dagger A_a|n\rangle. \end{aligned} \quad (12b)$$

Further simplification occurs when A is Hermitian. In that case we have

$$A_a{}^\dagger = (-1)^a A, \quad (13a)$$

and

$$\begin{aligned} S_n^{2a} &= (-1)^a\langle n|(A_a)^2|n\rangle, \\ S_n^{2a+1} &= \tfrac{1}{2}\langle n|(-1)^a A_a A_{a+1} + (-1)^{a+1}A_{a+1}A_a|n\rangle \\ &= \tfrac{1}{2}(-1)^a\langle n|[A_a,A_{a+1}]|n\rangle. \end{aligned} \quad (13b)$$

III. APPLICATIONS

We discuss some of the standard applications of the well-known sum rules (3); as well as develop new results from the general formulae (12) and (13).

A. It is evident from (13b) that to obtain the well-known sum rules for R_n^a; $a=0, 1, 2, 3, 4$; one needs only to know $A_0 = A$, and the first two commutants A_1, A_2. These sum rules may be quickly derived from (13b). Taking $A = x = A^\dagger$, and H given by (7), the first two commutants have a particularly simple form:

$$\begin{aligned} A_0 &= x, \\ A_1 &= (\hbar/im)p_x, \\ A_2 &= -\frac{\hbar^2}{m}\frac{\partial V}{\partial x}. \end{aligned} \quad (14a)$$

The sum rules for X_n^a defined by (2) (with an extra factor of $\hbar^{-a}$ when compared to S_n^a) are

$$\begin{aligned} X_n^0 &= \langle n|x^2|n\rangle, \\ X_n^1 &= \frac{1}{2im}\langle n|[x,p_x]|n\rangle = \left(\frac{\hbar}{2m}\right), \\ X_n^2 &= \frac{1}{m^2}\langle n|p_x^2|n\rangle, \\ X_n^3 &= \frac{i}{2m^2}\left\langle n\left|\left[p_x,\frac{\partial V}{\partial x}\right]\right|n\right\rangle = \frac{\hbar}{2m^2}\left\langle n\left|\frac{\partial^2 V}{\partial x^2}\right|n\right\rangle, \\ X_n^4 &= \frac{1}{m^2}\left\langle n\left|\left(\frac{\partial V}{\partial x}\right)^2\right|n\right\rangle. \end{aligned} \quad (14b)$$

Obviously the symmetric version of these results, R_n^a defined by (2), agrees with (3).

The general sum rule (13b) may be used to give sum rules for higher a. To calculate X_n^5, we need A_3 which is given by

$$A_3 = [H,A_2] = \frac{\hbar^3}{2m^2 i}\left[\mathbf{p}\cdot\nabla\frac{\partial V}{\partial x} + \nabla\frac{\partial V}{\partial x}\cdot\mathbf{p}\right]. \quad (15a)$$

Although A_3 is formidable, X_n^5 is still simple since it involves only the commutator of A_2 with A_3.

$$\begin{aligned} X_n^5 &= \frac{1}{2\hbar^5}\langle n|[A_2,A_3]|n\rangle \\ &= \frac{\hbar}{2m^3}\left\langle n\left|\left(\frac{\partial}{\partial x}\nabla V\right)^2\right|n\right\rangle \\ &= \frac{\hbar}{2m^3}\langle n|(\nabla F_x)^2|n\rangle \\ &= \frac{\hbar}{2m^3}\langle n|(\tfrac{1}{2}\nabla^2 F_x^2 - F_x\nabla^2 F_x)|n\rangle. \end{aligned} \quad (15b)$$

We have introduced the force $\mathbf{F} = -\nabla\mathbf{V}$. The symmetric sum is

$$R_n^5 = \frac{\hbar}{6m^3}\langle n|(\tfrac{1}{2}\nabla^2 F^2 - \mathbf{F}\cdot\nabla^2\mathbf{F})|n\rangle. \quad (15c)$$

Further sum rules for $a>5$ contain increasingly complicated expressions. Thus X_n^6 is

$$X_n^6=\frac{1}{4m^4}\langle n|(\mathbf{p}\cdot\nabla F_x+\nabla F_x\cdot\mathbf{p})^2|n\rangle. \tag{16}$$

Once some information about the potential V is available, the sum rules can yield an estimate for the behavior of $|\mathbf{r}_{kn}|^2$ when the energy $E(k)$ of the state k is large.

For example, for a central potential which is Coulombic at the origin, there is an argument (given, e.g., in Ref. 1) that utilizes the $a=3$ and $a=4$ sum rules, and that shows that if $E(k)$ is large and n is an s state, then $|\mathbf{r}_{kn}|^2$ varies as ω_{kn}^{-m}; $4<m\leqslant 5$. We apply this argument to the $a=4$ and $a=5$ sum rules to obtain a high-energy estimate for $|\mathbf{r}_{kn}|^2$ when n is a p state.

For a central potential which is Coulombic at the origin, we have at the origin

$$\begin{aligned} V&=\alpha/r,\\ \mathbf{F}&=\alpha\mathbf{r}/r^3,\\ (\nabla V)^2&=\alpha^2/r^4,\\ \tfrac{1}{2}\nabla^2F^2-\mathbf{F}\cdot\nabla^2\mathbf{F}&=\alpha^2\left[\frac{6}{r^6}-\frac{12\pi}{r^3}\delta(\mathbf{r})\right]. \end{aligned} \tag{17a}$$

At the origin, the radial wave function varies as r^l and the integrand of the radial integral arising in the evaluation of R_n^a behaves near the origin as

$$\begin{aligned} &r^{2l-2}, && (a=4)\\ &6r^{2l-4}-12\pi r^{2l-3}\delta(r), && (a=5). \end{aligned} \tag{17b}$$

Thus for $l=1$ p states, R_n^4 is finite but R_n^5 diverges because of the r^{-2} singularity at the origin. (We assume the potential is sufficiently well behaved away from the origin, so that no other singularities arise in the radial integration.) (Note that the delta function in the $a=5$ expression does not contribute when $l\geqslant 2$.) Returning now to the definition of R_n^a in terms of the infinite sums (2), we replace the high-energy, continuum contribution to the sum by an integral and assume that in this high-energy limit $|\mathbf{r}_{kn}|^2$ varies as ω_{kn}^{-m}. (The continuum wave functions are taken to be normalized on the energy scale.) Then for $l=1$, the sum rules state that

$$\begin{aligned} &\int^\infty \omega_{kn}^{4-m}d\omega_{kn} \quad \text{converges},\\ &\int^\infty \omega_{kn}^{5-m}d\omega_{kn} \quad \text{diverges}. \end{aligned} \tag{17c}$$

Hence $5<m\leqslant 6$. Explicit evaluation for a Coulomb potential when the state n is $2p$, gives $m=5.5$.

B. As a second application of (12b), we calculate sum rules of the form

$$B_n^a(q)=\sum_k \omega_{kn}^a|(e^{i\mathbf{q}\cdot\mathbf{r}})_{kn}|^2. \tag{18}$$

Taking $\mathbf{q}$ along the x axis and setting $B_0=e^{iqx}$, we have

$$\begin{aligned} B_0^\dagger B_0&=1,\\ B_1&=\tfrac{1}{2}iq\left[\frac{\hbar}{im}p_xB_0+B_0\frac{\hbar}{im}p_x\right]\\ &=B_0\left[iq\left(\frac{\hbar}{im}p_x\right)+\hbar q^2\left(\frac{\hbar}{2m}\right)\right]\\ &=B_0[iqA_1+\hbar q^2X_n^1],\\ B_1^\dagger&=[iqA_1+\hbar q^2X_n^1]B_0^\dagger. \end{aligned} \tag{19a}$$

We have expressed B_1 in terms of the quantities A_1 and X_n^1, defined in (14a) and (14b), respectively, which arise in connection with the dipole sum rules. The next commutant B_2 is

$$\begin{aligned} B_2&=B_0[(iqA_1+\hbar q^2X_n^1)^2+iqA_2],\\ B_2^\dagger&=[(iqA_1+\hbar q^2X_n^1)^2+iqA_2]B_0^\dagger. \end{aligned} \tag{19b}$$

The two commutants, B_1 and B_2, are sufficient to determine $B_n^a(q)$ for $a=0$, 1, 2, 3, 4. From (12b)

$$B_n^0(q)=\langle n|B_0B^\dagger{}_0|n\rangle=1, \tag{20a}$$

$$B_n^1(q)=\frac{1}{\hbar}\langle n|B_0^\dagger B_1|n\rangle=\frac{1}{\hbar}\langle n|iqA_1+\hbar q^2X_n^1|n\rangle. \tag{20b}$$

When the state n has definite parity, which we now assume, $\langle n|A_a|n\rangle$ vanishes since A_a is odd. Then B_n^1 becomes simply

$$B_n^1(q)=q^2X_n^1, \tag{20c}$$

$$\begin{aligned} B_n^2(q)&=\frac{1}{\hbar^2}\langle n|[iqA_1+\hbar q^2X_n^1]^2|n\rangle\\ &=q^2X_n^2+q^4(X_n^1)^2, \end{aligned} \tag{20d}$$

$$\begin{aligned} B_n^3(q)&=\frac{1}{\hbar^3}\langle n|(iqA_1+\hbar q^2X_n^1)^3\\ &\qquad+(iqA_1+\hbar q^2X_n^1)iqA_2|n\rangle\\ &=q^2X_n^3+3q^4X_n^2X_n^1+q^6(X_n^1)^3, \end{aligned} \tag{20e}$$

$$\begin{aligned} B_n^4(q)&=\frac{1}{\hbar^4}\langle n|[(iqA_1+\hbar q^2X_n^1)^2-iqA_2]\\ &\qquad\times[(iqA_1+\hbar q^2X_n^1)^2+iqA_2]|n\rangle\\ &=q^2X_n^4+q^4\left(\frac{\langle n|A_1^4|n\rangle}{\hbar^4}+4X_n^3X_n^1\right)\\ &\qquad+6q^6X_n^2(X_n^1)^2+q^8(X_n^1)^4. \end{aligned} \tag{20f}$$

We have used the dipole sums X_n^a, Eqs. (14), in the above.

$B_n^1(q)$ is Bethe's well-known generalization of the oscillator strength sum rule, which is important in calculating the energy loss of charged particles passing through matter.[1]

$B_n{}^a(q)$ for $a>4$ involves increasingly complicated expressions. However, it is evident that these expressions will always be expressible in terms of matrix elements of the commutants A_a arising in dipole sum-rule calculations. Also it is evident on dimensional grounds that $B_n{}^a(q)$ will be a polynomial in q^2 of order a (see also below). We may utilize this fact to obtain further sum rules by expanding both sides of (18) in powers of q and equating coefficients. We now proceed to do this.

Expanding $|(e^{i\mathbf{q}\cdot\mathbf{r}})_{kn}|^2=|(e^{iqx})_{kn}|^2$ gives

$$|(e^{iqx})_{kn}|^2=\sum_{m=0}^{\infty}(iq)^m c_m(k,n),$$

$$c_0(k,n)=\delta_{kn},$$

$$c_m(k,n)=\sum_{r=0}^{m}\frac{(-1)^r(x^r)_{nk}(x^{m-r})_{kn}}{r!(m-r)!}$$

$$=\frac{\delta_{kn}}{m!}[1+(-1)^m](x^m)_{nn}+\sum_{r=1}^{m-1}\frac{(-1)^r(x^r)_{nk}(x^{m-r})_{kn}}{r!(m-r)!}. \quad (21a)$$

When m is odd, the exponents r and $m-r$ are either even and odd, respectively, or odd and even, respectively. In either case $(x^r)_{nk}(x^{m-r})_{kn}$ vanishes by parity. Therefore $c_m=0$ for m odd. We may therefore, write (21a) as

$$|(e^{iqx})_{kn}|^2=\delta_{kn}\left[1-q^2(x^2)_{nn}+\sum_{m=2}^{\infty}(-1)^m q^{2m}\frac{2(x^{2m})_{nn}}{(2m)!}\right]+q^2|x_{kn}|^2+\sum_{m=2}^{\infty}(-1)^m q^{2m}d_m(k,n), \quad (21b)$$

$$d_m(k,n)=\sum_{r=1}^{2m-1}\frac{(-1)^r(x^r)_{nk}(x^{2m-r})_{kn}}{r!(2m-r)!}.$$

We now form the sums $B_n{}^a$. The $a=0$ case does not give any new result. For when $a=0$, we have according to (20a) and (21b)

$$1=\sum_k\delta_{kn}\left[1+\sum_{m=1}^{\infty}\frac{(-1)^m q^{2m}2(x^{2m})_{nn}}{(2m)!}\right]+q^2\sum_k|x_{kn}|^2+\sum_{m=2}(-1)^m q^{2m}\sum_{r=1}^{2m-1}\frac{(-1)^r}{r!(2m-r)!}\times\sum_k(x^r)_{nk}(x^{2m-r})_{kn}. \quad (22a)$$

Performing the k sums and grouping together powers of q^2 gives

$$0=\sum_{m=2}^{\infty}\frac{(-1)^m q^{2m}(x^{2m})_{nn}}{(2m)!}\left[2+\sum_{r=1}^{2m-1}\frac{(-1)^r(2m)!}{r!(2m-r)!}\right]. \quad (22b)$$

That (22b) is identically satisfied follows from the fact that

$$2+\sum_{r=1}^{2m-1}\frac{(-1)^r(2m)!}{r!(2m-r)!}=\sum_{r=0}^{2m}\frac{(-1)^r(2m)!}{r!(2m-r)!}=(1-1)^{2m}=0. \quad (22c)$$

Nontrivial results are obtained when $a>0$. In that case, the term in (21b) proportional to δ_{kn} does not contribute since $\sum_k\omega_{kn}{}^a\delta_{kn}=\omega_{nn}{}^a=0$ when $a>0$. From (21b) we have

$$B_n{}^a(q)=\sum_k\omega_{kn}{}^a|(e^{iqx})_{kn}|^2=q^2X_n{}^a+\sum_{m=2}(-1)^m q^{2m}\sum_k\omega_{kn}{}^a d_m(k,n). \quad (23)$$

It is seen that $B_n{}^a$ contains a term $q^2X_n{}^a$. This has been explicitly demonstrated for $a=1$, 2, 3, 4; see Eqs. (20).

According to previous remarks, $B_n{}^a(q)$ is a polynomial in q^2 of order a. Hence the coefficients of q^{2m} in (23) must vanish for $m>a$. Therefore we can give the sum rule

$$\sum_k\omega_{kn}{}^a d_m(k,n)=0,\quad m>a\geqslant 1. \quad (24)$$

When explicit expressions for $B_n{}^a(q)$ are available, as in Eqs. (20) for $a=1$, 2, 3, 4, the coefficients of q^{2m}, $m\leqslant a$, in Eq. (23) can be evaluated. Thus combining (23) with (20), we have

$$(X_n{}^1)^2=\frac{\hbar^2}{4m^2}=\sum_k\omega_{kn}{}^2d_2(k,n), \quad (25a)$$

$$3X_n{}^2X_n{}^1=\sum_k\omega_{kn}{}^3d_2(k,n), \quad (25b)$$

$$\frac{\langle n|A_1{}^4|n\rangle}{\hbar^4}+4X_n{}^3X_n{}^1=\sum_k\omega_{kn}{}^4d_2(k,n), \quad (25c)$$

$$(X_n{}^1)^3=\frac{\hbar^3}{8m^3}=-\sum_k\omega_{kn}{}^3d_3(k,n), \quad (25d)$$

$$6X_n{}^2(X_n{}^1)^2=-\sum_k\omega_{kn}{}^4d_3(k,n), \quad (25e)$$

$$(X_n{}^1)^4=\frac{\hbar^4}{16m^4}=\sum_k\omega_{kn}{}^4d_4(k,n). \quad (25f)$$

It is striking that some of the above sum rules, Eqs. (25a), (25d), and (25f), give a result independent of the state n. When the oscillator-strength sum rule, which also gives a result independent of the state n, is written in the present notation, it takes on the form

$$X_n{}^1=\frac{\hbar}{2m}=-\sum_k \omega_{kn}d_1(k,n)\,. \qquad (26a)$$

Comparing this to (25a), (25d), and (25f), the following generalization suggests itself

$$(X_n{}^1)^a=\left(\frac{\hbar}{2m}\right)^a=(-1)^a\sum_k \omega_{kn}{}^a d_a(k,n)\,. \qquad (26b)$$

To establish (26b) we first prove that

$$B_a=B_0\{(\hbar q^2X_n{}^1)^a+O(q^{2a-1})\}\,. \qquad (27a)$$

We prove (27a) inductively. For $a=1$ it is true, see (19a). Then, assuming (27a) for B_a,

$$\begin{aligned}B_{a+1}&=[H,B_a]=[H,B_0\{(\hbar q^2X_n{}^1)^a+O(q^{2a-1})\}]\\&=B_1\{(\hbar q^2X_n{}^1)^a+O(q^{2a-1})\}\,.\end{aligned} \qquad (27b)$$

Inserting B_1 from (19a) gives

$$B_{a+1}=B_0\{(\hbar q^2X_n{}^1)^{a+1}+O(q^{2a+1})\}\,, \qquad (27c)$$

which establishes (27a). Next we use (10) to evaluate $B_n{}^a(q)$

$$B_n{}^a(q)=\frac{1}{\hbar^a}\langle n|B_0{}^\dagger B_a|n\rangle=q^{2a}(X_n{}^1)^a+O(q^{2a-1})\,. \qquad (27d)$$

Comparing this to the expansion of $B_n{}^a(q)$ in powers of q^2, given in (23), gives the result (26b). Thus (26b) is indeed true and provides a generalization of the oscillator-strength sum rule.

We conclude this discussion of the sum rules for $B_n{}^a(q)$ with the remark that the result that $B_n{}^1(q)$ is correctly given by the dipole approximation to e^{iqx}, see (20c), is well known[1] and plays an important role in Bethe's theory of the energy loss of a charged particle passing through matter.[1] This fact, which is somewhat mysterious when taken in isolation, is seen to be a special case of our formula (24).

C. As a final application of the general sum rules (12) we note that (12a) gives several, formally different, expressions for $S_n{}^a$. Further, formally different, expressions are obtained by taking linear combinations of these. By utilizing the fact that n is an energy eigenstate, we showed that all these expressions are identical [cf. Eqs. (11)]. However, frequently the exact eigenfunction is unknown and only approximate wave functions are available. With an approximate wave function, the various expressions for $S_n{}^a$ of course are no longer identical. One may therefore test the accuracy of the approximate wave function by examining the discrepancies between the various expressions for $S_n{}^a$. In particular, if one can persuade oneself that the various expressions for $S_n{}^a$ test different parts of the wave function one can determine where the approximate wave function is inaccurate. For example in calculating $S_n{}^3$, with an approximate wave function u_n, we have four expressions:

$$\begin{aligned}S_n{}^3(1)&=\int u_n{}^*(\mathbf{r})A^\dagger A_3u_n(\mathbf{r})d\mathbf{r}\,,\\S_n{}^3(2)&=\int u_n{}^*(\mathbf{r})A_1{}^\dagger A_2u_n(\mathbf{r})d\mathbf{r}\,,\\S_n{}^3(3)&=\int u_n{}^*(\mathbf{r})A_2{}^\dagger A_1u_n(\mathbf{r})d\mathbf{r}\,,\\S_n{}^4(4)&=\int u_n{}^*(\mathbf{r})A_3{}^\dagger Au_n(\mathbf{r})d\mathbf{r}\,.\end{aligned} \qquad (28)$$

Suppose $A^\dagger A_3$ and $A_3{}^\dagger A$ are large only for small r, while $A_1{}^\dagger A_2$ and $A_2{}^\dagger A_1$ are large only for large r. If there is a significant discrepancy between $S_n{}^3(1)$ and $S_n{}^3(4)$, but not between $S_n{}^3(2)$ and $S_n{}^3(3)$, we may conclude that u_n is inaccurate for small r.

This procedure becomes particularly effective, if it can be shown that $S_n{}^a$ does not depend on the wave function. This may happen independent of the form of Hamiltonian, as in the oscillator sum rule. It may also happen because of the fortuitous nature of the potential. For example $R_n{}^3$ and $R_n{}^5$ do not depend on the wave function when the potential is a harmonic oscillator. With the general sum rules that we have derived, given a potential, it may be possible to construct an expression which does not depend on the wave function.

IV. GENERALIZATION

In this section we examine to what extent the general methods for sum rules, developed in II, can be applied to sums which are weighted by a negative power of the energy difference.

$$S_n{}^{-a}=\sum_k{}' (E_k-E_n)^{-a}|A_{kn}|^2\,, \qquad (29)$$

where $a=1, 2, \cdots$. The prime on the sum indicates that all states m with $E_m=E_n$ are omitted.

We first concern ourselves with the $a=1$ case. The general formula (10) for $S_n{}^a$ suggest an expression for $S_n{}^{-1}$,

$$S_n{}^{-1}=\sum_k (E_k-E_n)^{-1}|A_{kn}|^2\overset{(?)}{=}\langle n|A^\dagger A_{-1}|n\rangle\,, \qquad (30a)$$

where the inverse commutant A_{-1} is defined by

$$[H,A_{-1}]=A_0=A\,. \qquad (30b)$$

Taking matrix elements of (30b) gives

$$(E_k-E_n)\langle k|A_{-1}|n\rangle=\langle k|A|n\rangle\,. \qquad (30c)$$

Inserting a complete set of states in the right-hand side of (30*a*) gives

$$\begin{aligned}\langle n|A^\dagger A_{-1}|n\rangle=&\sum_k{}' \langle n|A^\dagger|k\rangle\langle k|A_{-1}|n\rangle\\&+\sum_m \langle n|A^\dagger|m\rangle\langle m|A_{-1}|n\rangle\,.\end{aligned} \qquad (30d)$$

We have separated the sum over all states into a sum over the states k for which $E_k \neq E_n$, and another sum over the states m for which $E_m = E_n$. In the first sum, $\langle k|A_{-1}|n\rangle$ may be evaluated from (30c). However in the second sum, we cannot evaluate $\langle m|A_{-1}|n\rangle$, since (30c) does not determine $\langle m|A_{-1}|n\rangle$ when $E_m = E_n$. Then (30d) becomes

$$\langle n|A^\dagger A_{-1}|n\rangle - \sum_m \langle n|A^\dagger|m\rangle\langle m|A_{-1}|n\rangle = \sum_k{}' \frac{\langle n|A^\dagger|k\rangle\langle k|A|n\rangle}{E_k - E_n} = S_n^{-1}. \quad (30e)$$

Thus it is seen that the correct formula for S_n^{-1} is not (30a), but (30e).

We now prove the general result

$$S_n^{-a} = \langle n|A^\dagger A_{-a}|n\rangle - \sum_m \langle n|A^\dagger|m\rangle\langle m|A_{-a}|n\rangle, \quad (31a)$$

where the inverse commutant is defined recursively by

$$[H, A_{-a}] = A_{-a+1}. \quad (31b)$$

To prove (31a) we first establish by induction that

$$(E_k - E_n)^a \langle k|A_{-a}|n\rangle = \langle k|A|n\rangle. \quad (32a)$$

According to (30c), (32a) is true for $a=1$. We assume it true for a. For $a+1$ we have

$$\begin{aligned} [H, A_{-a-1}] &= A_{-a}, \\ (E_k - E_n)\langle k|A_{-a-1}|n\rangle &= \langle k|A_{-a}|n\rangle, \\ (E_k - E_n)^{a+1}\langle k|A_{-a-1}|n\rangle &= (E_k - E_n)^a\langle k|A_{-a}|n\rangle \\ &= \langle k|A|n\rangle, \end{aligned} \quad (32b)$$

which establishes (32a). Inserting a complete set of states in $\langle n|A^\dagger A_{-a}|n\rangle$ yields

$$\begin{aligned} \langle n|A^\dagger A_{-a}|n\rangle - \sum_m \langle n|A^\dagger|m\rangle\langle m|A_{-a}|n\rangle &= \sum_k{}' \langle n|A^\dagger|k\rangle\langle k|A_{-a}|n\rangle \\ &= \sum_k{}' \frac{\langle n|A^\dagger|k\rangle\langle k|A|n\rangle}{(E_k - E_n)^a} = S_n^{-a}. \end{aligned} \quad (32c)$$

This proves (31a).

Again we may give several, formally different, expressions for S_n^{-a} by using the fact that

$$\langle n|A_{-b}{}^\dagger A_{-a+b}|n\rangle = \langle n|A^\dagger A_{-a}|n\rangle. \quad (33a)$$

To prove (33a) we proceed as in II

$$\begin{aligned} \langle n|A^\dagger A_{-a}|n\rangle &= \langle n|[H, A_{-1}]^\dagger A_{-a}|n\rangle \\ &= \langle n|(A_{-1})^\dagger H A_{-a} - H(A_{-1})^\dagger A_{-a}|n\rangle \\ &= \langle n|(A_{-1})^\dagger (HA_{-a} - A_{-a}H)|n\rangle \\ &= \langle n|(A_{-1})^\dagger A_{-a+1}|n\rangle. \end{aligned} \quad (33b)$$

Continuing this procedure b times gives (33a). Thus the simplest expression for S_n^{-a} is

$$\begin{aligned} S_n^{-2a} &= \langle n|A_{-a}{}^\dagger A_a|n\rangle - \sum_m \langle n|A^\dagger|m\rangle \times \langle m|A_{-2a}|n\rangle, \\ S_n^{-(2a+1)} &= \langle n|A_{-a}{}^\dagger A_{-a-1}|n\rangle - \sum_m \langle n|A^\dagger|m\rangle \times \langle m|A_{-2a-1}|n\rangle \\ &= \langle n|A_{-a-1}{}^\dagger A_{-a}|n\rangle - \sum_m \langle n|A^\dagger|m\rangle \times \langle m|A_{-2a-1}|n\rangle. \end{aligned} \quad (34)$$

The inverse commutants A_{-a}, defined by (31b), are not unique, as any constant of motion, which commutes with the Hamiltonian, may be added to A_{-a}. Since a constant of motion has zero-valued matrix elements between states of different energy, this nonuniqueness does not affect the final result.

If $\langle m|A|n\rangle$ is nonzero, where m is a state with energy E_n, (32a) shows that $\langle m|A_{-a}|n\rangle$ diverges. Thus, the right-hand side of (34) is the difference of two infinite quantities, and care must be exercised in an evaluation. If $\langle m|A|n\rangle$ vanishes, then $\langle m|A_{-a}|n\rangle$ can be finite, and the subtracted sums on the right-hand side of (34) vanish.

Although we have succeeded in giving a closed form for S_n^{-a}, expressions (34), these are rarely of practical value since in general one cannot calculate the inverse commutants A_{-a}. For the particularly simple case of a harmonic oscillator, A_{-a} can be obtained when $A = x$. However the sum S_n^{-a} can just as easily be calculated directly in that case, because of the simple nature of the matrix elements of x.[3]

[3] Special cases of our formula (32c) have been derived by A. Dalgarno and J. T. Lewis, Proc. Roy. Soc. (London) **A233**, 70 (1956). C. Schwartz [Ann. Phys. (N. Y.) **6**, 156 (1959)] applied the results of Dalgarno and Lewis to obtain approximate results for sums of the kind discussed in part IV of the present paper.