

LETTER TO THE EDITOR

The Thomas-Reiche-Kuhn sum rule for an atom of N equally spaced energy levels

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Abstract. The Thomas-Reiche-Kuhn sum rule is determined for an atom consisting of an arbitrary number of discrete, equally spaced eigenenergy levels. This generalization is consistent with a two-level atom and with a usually seen form of the sum rule involving the atomic ground state, and resolves an apparent paradox reported elsewhere.

The Thomas-Reiche-Kuhn (TRK) sum rule may be written in the form

$$\sum_n \{\omega_I + \omega_J - 2\omega_n\} \langle I|q|n\rangle \langle n|q|J\rangle = -\frac{\hbar}{m} \delta_{IJ} \quad (1)$$

for a one-dimensional, bound system. This equation relates the matrix elements of the position q of the electron (of mass m) with the eigenenergies $\hbar\omega_x = E_x$ and orthonormal eigenstates $|x\rangle$ of the atomic Hamiltonian H , where $x = I, J$ or n . The summation over n involves an infinite number of all possible levels, consistent with the infinite dimensionality of the state space. Equation (1) may be determined from the imposition of the closure relationship $\sum_{n=0}^{\infty} |n\rangle \langle n| = 1$ on the expression $\langle I|[q, [q, H]]|J\rangle$. The TRK sum rule, which is more usually given in the special form

$$\sum_n (E_n - E_0) |\langle 0|q|n\rangle|^2 = \frac{\hbar^2}{m} \quad (2)$$

(Orlandini and Traini 1991) involving the atomic ground state $|0\rangle$, may be re-expressed in terms of matrix elements involving the electronic momentum p from the relationship

$$\langle A|p|B\rangle = im\{\omega_A - \omega_B\} \langle A|q|B\rangle \quad (3)$$

where A, B designate any two atomic levels. In an infinite dimensional state space, the conjugate variables q and p form the canonical commutator $[q, p] = i\hbar$. The extensions of the formalism to a three-dimensional atom of general atomic number are trivial.

The TRK sum rule (1) is inconsistent with a two-level atom, since its application to the ground $|0\rangle$ and excited $|1\rangle$ states gives

$$|\langle 0|q|1\rangle|^2 = \hbar/2m\omega \quad |\langle 1|q|0\rangle|^2 = -\hbar/2m\omega \quad (4)$$

respectively; where $\hbar\omega$ is the energy separation between the two atomic levels—that is, $E_0 = 0$ and $E_1 = \hbar\omega$. This has been thought to indicate an inadequacy in the two-level model, particularly in calculations of atomic energy shifts near to boundaries (Barton 1974). On the other hand, the application of the TRK sum rule in the form of (2) to

quantum electrodynamical calculations involving a two-level atom seems to be successful (Jhe 1991). The resolution of the apparent paradox lies in the fact that (1) is an incorrect form of the TRK sum rule in the case of an atom composed a finite number of eigenenergy levels. The finite dimensionality of the state space must be taken into account, and this results in a modification to the right-hand side of (1).

The application of closure in the form $\sum_{n=0}^s |n\rangle\langle n| = 1$ leads to the relationship

$$\langle i|[q_s, [q_s, H_s]]|j\rangle = \hbar\omega \sum_{n=0}^s \{i+j-2n\}\langle i|q|n\rangle\langle n|q|j\rangle \quad (5)$$

involving any two orthonormal, energy eigenstates $|i\rangle$ and $|j\rangle$ of an $N = s+1$ level, one-dimensional bound system. Here, q_s denotes the position of the electron and $\hbar\omega$ is the uniform energy separation between adjacent levels. The restriction of the discussion to N equally spaced energy levels is justified by the subsequent specialization to a system of only two levels. The atomic Hamiltonian $H_s = \hbar\omega \sum_n n|n\rangle\langle n|$ may be expressed in terms of

$$\pi_s = \sum_{n=0}^{s-1} (n+1)^{1/2}|n\rangle\langle n+1| \quad \pi_s^\dagger = \sum_{n=0}^{s-1} (n+1)^{1/2}|n+1\rangle\langle n| \quad (6)$$

as

$$H_s = \hbar\omega \pi_s^\dagger \pi_s. \quad (7)$$

The operators (6) have the usual raising and lowering ladder properties

$$\begin{aligned} \pi_s|m\rangle &= m^{1/2}|m-1\rangle & m \neq 0 & & \pi_s|0\rangle &= 0 \\ \pi_s^\dagger|m\rangle &= (m+1)^{1/2}|m+1\rangle & m \neq s & & \pi_s^\dagger|s\rangle &= 0. \end{aligned} \quad (8)$$

The commutator

$$[\pi_s, \pi_s^\dagger] = 1 - (s+1)|s\rangle\langle s| \quad (9)$$

reflects the arbitrary dimensionality of the atomic state space. In the divergent $N \rightarrow \infty$ limit, equation (9) assumes to any finite degree of accuracy the bosonic form of a unit matrix, corresponding to a harmonic oscillator, in a manner similar to that described in a different context by Barnett and Pegg (1989). A pair of conjugate operators

$$q_s = f\pi_s + f^*\pi_s^\dagger \quad p_s = \frac{i}{\hbar} [H_s, mq_s] = -im\omega\{f\pi_s - f^*\pi_s^\dagger\} \quad (10)$$

may be constructed from the use of (7) and (9), where $f = \langle 0|q_s|1\rangle$ and $f^* = \langle 1|q_s|0\rangle$. The commutator $[q_s, p_s] = i\hbar[\pi_s, \pi_s^\dagger]$ becomes canonical in the limit $N \rightarrow \infty$, allowing the identification $|f|^2 = \hbar/2m\omega$ to be made. Therefore from (9), (10) the equation

$$[q_s, [q_s, H_s]] = -\frac{\hbar^2}{m} \{1 - (s+1)|s\rangle\langle s|\} \quad (11)$$

may be written down, leading to the form

$$\sum_{n=0}^s \omega\{i+j-2n\}\langle i|q_s|n\rangle\langle n|q_s|j\rangle = -\frac{\hbar}{m} \{\delta_{ij} - (s+1)\delta_{is}\delta_{sj}\} \quad (12)$$

of the generalized TRK sum rule for an atom composed of $N = s+1$ equally spaced levels. This constitutes the main result of the work reported here. It should be noted that the generalized TRK sum rule (12) may be written in the special form (2) for

general non-zero s , and, in the limit $N \rightarrow \infty$, corresponding to a harmonic oscillator, the usual sum rule (1) is recovered. There is no inconsistency involving (12) when applied to a two-level atom, since, dropping the s subscripts, $|\langle 0|q|1\rangle|^2 = |\langle 1|q|0\rangle|^2 = \hbar/2m\omega$. Equation (12) may also be expressed in terms of matrix elements involving the momentum p_s , because (3) is valid for all N .

In conclusion, the TRK sum rule has been generalized to a form (12) appropriate to a uniformly spaced N -level atom; one, which, although different from the rule (1) obtained in the case of an infinitely dimensional state space, may, since $s > 0$, be specialized to an often used form (2) involving the atomic ground state. Furthermore, there is no inconsistency between the generalized TRK sum rule and a two-level atom.

References

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