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Sum rules for the quarkonium systems

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In the framework of the radial Schrödinger equation we derive in a very simple way sum rules relating the potential to physical quantities such as the energy eigenvalues and the square of the lth derivative of the eigenfunctions at the origin. These sum rules contain as particular cases well-known results such as the quantum version of the Clausius theorem in classical mechanics as well as Kramers's relations for the Coulomb potential. Several illustrations are given and the possibilities of applying them to the quarkonium systems are considered.

I. INTRODUCTION

The discovery of the ψ in 1974[1] and the subsequent observations of the ψ-like particle spectrum during 1975[2] suggested strongly that those new particles can be described as a nearly nonrelativistic bound system of charmed quark and antiquark.[3] Charmonium, as this $q\bar{q}$ bound state was soon called, has been extensively used in the phenomenological interpretation of the different properties of the psion family.[3-4] Nowadays, several factors have increased the interest of this "naive" model. On the experimental side, the discovery of the Υ particles[5] and the conviction that they are associated with a still heavier quark, the b quark, has led to the introduction, by analogy with charmonium, of the b-quark–antiquark system. If charmonium is marginally nonrelativistic, we expect $b\bar{b}$ to be fully nonrelativistic since m_b is about three times larger than m_c. On the theoretical side we have more and more indications that forces between quarks depend on colors and not on flavors. Therefore if some type of potential is successful in charmonium, essentially *the same potential* should also be successful in $b\bar{b}$.[6] The model gets in that way *more predictive power*. Finally, it is largely recognized that the simplest model which can account *naturally*[7] for CP-violating forces must at least contain six quarks.[8] The sixth quark called the t quark, has a mass equal to or greater than 10 GeV.[9] It should also generate a whole new family of particles which can be described as $t\bar{t}$ nonrelativistic bound states.

What is the potential to be used? The answer to that question is not yet known and is expected to be very difficult. From quantum chromodynamics (QCD) we can make two qualitative arguments: First, when the distance r between the quark and the antiquark is small, say $r < 0.2$ fm, asymptotic freedom tells us that the spin-independent part of $V(r)$ should be

$$V(r) \approx -\frac{4}{3}\frac{\alpha_s(r)}{r},$$

where $\alpha_s(r)$ is the running coupling constant. The spin-dependent part is also calculable and different from zero. Second, when the distance between the quark and the antiquark is large, say $r \gtrsim 0.8$ fm, forces become strong, confining, and essentially spin independent.[10] Qualitative arguments suggest that this potential could rise linearly with the distance.[11] It should be stressed that since confinement is not yet proved in QCD,[12] this last statement is quite uncertain. From our present experience with the charmonium model, we know that the mean radius of ψ is about 0.5 fm, i.e., a distance where both short-range forces and confining forces are expected to play a role. Around this distance there is no basic understanding of the nature of the potential. Therefore, we deal, in the context of charmonium, with an inverse problem which can be stated as follows: From the experimental spectrum, from transition rates, and from decay probabilities *deduce* the form of the potential. This problem looks very old fashioned[13] but here it has a very novel feature which we would like to stress. Heavy vector particles such as ψ, ψ', Υ, Υ', etc., considered as bound $Q\bar{Q}$ systems resemble the hydrogen atom but *at the same time* they can decay in a similar way to the positronium which is a relativistic system. It then follows that the value of the modulus squared of the wave function or of some of its derivatives at the origin *takes on a physical meaning*. This together with the confining nature of the potential has led Quigg, Rosner, and Thacker[14] and Grosse and Martin[15] to reformulate the inverse problem for the $l = 0$ states in a very efficient way. In this reformula-

tion the value of $|\psi_n(0)|^2$ for each level n plays a leading part. On a more modest level, the use of sum rules has proved to be very useful in estimating the behavior of physical quantities or to constrain the potential without the need to solve the Schrödinger equation.

Up to now two sum rules have been used. The first one relates $|\psi_n(0)|^2$ to the mean value of the derivative of the potential $V'(r)$, and has been known for many years.[16] The second one is the quantum-mechanical expression of the Clausius theorem in classical mechanics.[17] It has been rederived recently by Martin[18] from direct manipulations of the Schrödinger equation.

The present work is an investigation of sum rules both from the point of view of their derivation and of their use. Specifically we show that the sum rules already used are particular cases of much more general sum rules. We propose a simple procedure to derive them. We show that they are valid for any value of the angular momentum. We illustrate by several examples how they can be utilized to discuss the physical properties of quarkonium and to obtain constraints on the potential.

In Sec. II we define our notations and conventions. In Sec. III we show through an example that the hypervirial theorems[19] must be handled very carefully to avoid inconsistencies. We propose a constructive way to avoid this. Finally we show how to deduce sum rules. In Sec. IV we illustrate the context of the sum rules through many examples. In particular, we show how to recover already known sum rules including Kramers's relations for the Coulomb problem. We also derive new sum rules relevant for the study of quarkonium systems. We conclude with a few remarks on their usefulness and make suggestions for further developments.

To close this Introduction, let us stress that we concentrate in this work on the radial-wave Schrödinger equation neglecting spin-spin, spin-orbit, and tensor forces. This is not an essential restriction but it is done in order not to confuse the main points of this paper.

II. NOTATIONS AND CONVENTIONS

The three-dimensional wave function is written

$$\psi(\vec{r}) = \tilde{R}(r) Y_{lm}(\theta, \phi), \tag{2.1}$$

with the normalization conditions

$$\int |\psi(\vec{r})|^2 d^3r = 1, \tag{2.2}$$

$$\int d\Omega\, Y^*_{lm}(\theta, \phi) Y_{l'm'}(\theta, \phi) = \delta_{ll'}\delta_{mm'}, \tag{2.3}$$

$$\int_0^\infty |\tilde{R}(r)|^2 r^2 dr = 1. \tag{2.4}$$

The radial wave function is written

$$u(r) = r\tilde{R}(r). \tag{2.5}$$

We introduce the scaled distance variable

$$\rho = \alpha r, \tag{2.6}$$

where α is any constant with the dimension of a mass. As we shall see later on, the form of α can vary with the specific physical features of the interaction. Going from the r variable to the ρ variable the radial wave function can be written successively as

$$u(r) = r\tilde{R}(r) = \frac{\rho}{\alpha}\tilde{R}\left(\frac{\rho}{\alpha}\right) = \rho R(\rho) = w(\rho). \tag{2.7}$$

Therefore the normalization condition for $w(\rho)$ is

$$\int_0^\infty |w(\rho)|^2 d\rho = \alpha. \tag{2.8}$$

The Schrödinger equation for $w(\rho)$ is

$$H(\rho) w(\rho) = e w(\rho), \tag{2.9}$$

with

$$H(\rho) = -\frac{d^2}{d\rho^2} + U(\rho), \tag{2.10}$$

$$U(\rho) = \frac{l(l+1)}{\rho^2} + V(\rho), \tag{2.11}$$

$$V(\rho) = 2\mu\alpha^{-2}\tilde{V}\left(\frac{\rho}{\alpha}\right), \tag{2.12}$$

and

$$e = 2\mu\alpha^{-2}E. \tag{2.13}$$

In Eqs. (2.12) and (2.13), $\tilde{V}(r)$ and E are the usual expressions of the potential and of the energy eigenvalue. Whenever it is needed we explicitly display the quantum numbers, which label each eigenfunction, and denote them by n and l, i.e.,

$$w(\rho) \to w_{nl}(\rho). \tag{2.14}$$

If a wave function is not necessarily an eigenfunction of H we denote it by a symbol *different from* w. The Dirac notation for $w_{nl}(\rho)$ is $|nl\rangle$ or $|m\rangle$, when we do not need to display the angular momentum, or simply $|w\rangle$, when we do not need to display quantum numbers. Finally we write for any operator $G(\rho)$

$$\langle G(\rho)\rangle = \frac{\langle m|G(\rho)m\rangle}{\langle m|m\rangle} = \frac{1}{\alpha}\int_0^\infty w^*_m(\rho) G(\rho) w_m(\rho) d\rho. \tag{2.15}$$

It should be stressed that $G(\rho)$ is not symmetric (or Hermitian) in general. In order to stress that

$G(\rho)$ must always be applied to the ket vector and not to the bra vector, we write $\langle m|G(\rho)m\rangle$ for its matrix element instead of the usual notation $\langle m|G(\rho)|m\rangle$.

III. THE DERIVATION OF SUM RULES

It is a well known fact that sum rules can be deduced from the hypervirial theorems.[19] However, these theorems, as they are usually stated, involve an implicit assumption, namely, that the Hamiltonian matrix elements are always symmetric, i.e., $\langle f|Hg\rangle = \langle g|Hf\rangle^*$. Since the domain of Hilbert space, in which it is indeed the case, is not explicitly given, it is easy to find examples where these theorems are *violated*. In a separate article, we have examined the mathematical problem in itself.[20] In this section we merely propose a way to avoid the difficulties. Basically we show that the violation of the hypervirial theorems is always connected with the appearance of *boundary terms*. Once these boundary terms are taken into account, they lead to a modified form of the hypervirial theorems out of which *sum rules can again be deduced*. First we remind the reader how hypervirial theorems can be stated in the context of the radial wave Schrödinger equation: If W is a time-independent operator function of ρ and $d/d\rho$ then

$$\langle m|[H,W]|m\rangle = 0 . \tag{3.1}$$

It is obvious that whenever H is supposed to be symmetric the right-hand side is indeed zero. However, the following example shows that it is *often not the case*.

Take

$$W = \frac{d}{d\rho} , \tag{3.2}$$

then

$$[H,W] = \left[H, \frac{d}{d\rho}\right] = -U^{(1)}(\rho) . \tag{3.3}$$

Therefore, (3.1) implies

$$\langle m|U^{(1)}(\rho)|m\rangle = 0 . \tag{3.4}$$

This relation is certainly not true in general since, for instance, when

$$U(\rho) = \lambda\rho , \tag{3.5}$$

(3.4) implies

$$\langle m|m\rangle = 0 . \tag{3.6}$$

The only reason we arrive at this inconsistency is that

$$\left\langle m\left| H\frac{d}{d\rho}\right|m\right\rangle = e_m\left\langle m\left|\frac{d}{d\rho}\right|m\right\rangle \tag{3.7}$$

is not always true. This is the case when $l=0$ because the state

$$|f\rangle = \frac{d}{d\rho}|m\rangle \tag{3.8}$$

is such that $f(\rho=0)\neq 0$. Therefore (3.7) is violated by a *boundary term*.[21] Next we show how it is possible in all cases of physical interest to extract boundary terms.[20]

Definition. We introduce the sesquilinear form

$$\langle g|Hf\rangle = \int_0^\infty g^*(\rho)[(Hf)(\rho)]d\rho . \tag{3.9}$$

Then

$$\langle Hg|f\rangle = \int_0^\infty [(Hg)(\rho)]^* f(\rho)d\rho . \tag{3.10}$$

Theorem. If $|w\rangle$ is an eigenfunction of H and if $f(\rho)$ is such that

$$\langle w|Hf\rangle = \int_0^\infty w^*(\rho)(Hf)(\rho)d\rho < \infty , \tag{3.11}$$

we can always write

$$\langle w|Hf\rangle = \langle f|Hw\rangle^* + 2\left\langle w\left|\left\{\frac{d}{d\rho}, \delta(\rho)\right\}\right|f\right\rangle . \tag{3.12}$$

This formula plays a crucial role in our derivation of sum rules. It is interesting because each term can be given a well-defined mathematical meaning. The boundary term is the matrix element of a well defined operator[20]

$$K(\rho) = 2\left\{\frac{d}{d\rho}, \delta(\rho)\right\} . \tag{3.13}$$

Obviously whenever f is in the domain where H is symmetric[22] we always have

$$\langle w|K(\rho)|f\rangle = 0 . \tag{3.14}$$

Formula (3.12) is not mysterious. It is only a convenient way to write the partial-integration formula. To see that, we notice first that it is enough to consider $H_0 = -d^2/d\rho^2$, because whenever $U(\rho)$ is real the form $\langle w|Uf\rangle$ is always symmetric. Starting from $\langle w|H_0 f\rangle$ and doing two successive partial integrations we find

$$\langle w|H_0 f\rangle = \langle f|H_0 w\rangle^* + \left[w^*\frac{d}{d\rho}f - \left(\frac{d}{d\rho}w^*\right)f\right]_{\rho=0} . \tag{3.15}$$

Writing the boundary term as a matrix element leads immediately to (3.12). From (3.12) it follows that the hypervirial theorems (3.1) can be written in the following generalized form:

$$\langle m|[H,W]|m\rangle = +2\left\langle m\left|\left\{\frac{d}{d\rho}, \delta(\rho)\right\}W\right|m\right\rangle . \tag{3.16}$$

This formula allows us to consider all operators W such that $W|m\rangle$ *does not belong* to the domain in the Hilbert space inside which the Hamiltonian H is symmetric. Before we proceed further, let us notice that we can also consider off-diagonal elements of $[H, W]$ without difficulty. If $|m\rangle$ and $|m'\rangle$ are two different eigenstates then (3.16) becomes

$$\langle m|[H,W]|m'\rangle = (e_m - e_{m'})\langle m|W|m'\rangle + 2\left\langle m\left|\left\{\frac{d}{d\rho}, \delta(\rho)\right\}W\right|m'\right\rangle . \tag{3.16'}$$

A. Sum rules

We shall deduce from (3.16) sum rules which appear to have a physical interest. Since many choices of W are possible, there are also several ways to deduce them. We present here the simplest one. Let us choose

$$W(\rho) = g(\rho)\frac{d}{d\rho} . \tag{3.17}$$

In order to satisfy (3.11) we assume that $g(\rho)$ does not increase exponentially. We compute the commutator $[H, W]$ and we find

$$\left[H, g(\rho)\frac{d}{d\rho}\right] = -g^{(2)}(\rho)\frac{d}{d\rho} + 2g^{(1)}(\rho)H - 2g^{(1)}(\rho)U(\rho) - g(\rho)U^{(1)}(\rho) , \tag{3.18}$$

where the upper indices indicate the order of the derivatives. The left-hand side of (3.16) is

$$\left\langle m\left|\left[H, g(\rho)\frac{d}{d\rho}\right]\right|m\right\rangle = -\left\langle m\left|g^{(2)}(\rho)\frac{d}{d\rho}m\right\rangle + 2e_m\langle m|g^{(1)}(\rho)m\rangle - 2\langle m|g^{(1)}(\rho)U(\rho)m\rangle - \langle m|g(\rho)U^{(1)}(\rho)m\rangle . \tag{3.19}$$

The right-hand side can be computed directly. The result is

$$2\left\langle m\left|\left\{\frac{d}{d\rho}, \delta(\rho)\right\}g(\rho)\frac{d}{d\rho}\right|m\right\rangle = -\lim_{\rho\to 0}\left[g(\rho)|w_m^{(1)}(\rho)|^2 - g(\rho)w_m^*(\rho)w_m^{(2)}(\rho) - g^{(1)}(\rho)w_m^*(\rho)w_m^{(1)}(\rho)\right] . \tag{3.20}$$

Equations (3.16), (3.19), and (3.20) lead to the following (infinite) set of sum rules:

$$-2e_m\langle m|g^{(1)}(\rho)m\rangle + 2\langle m|g^{(1)}(\rho)U(\rho)m\rangle + \left\langle m\left|g^{(2)}(\rho)\frac{d}{d\rho}m\right\rangle + \langle m\left|g(\rho)U^{(1)}(\rho)m\right\rangle = \lim_{\rho\to 0}\left[g(\rho)|w_m^{(1)}(\rho)|^2 - g(\rho)w_m^*(\rho)w_m^{(2)}(\rho) - g^{(1)}(\rho)w_m^*(\rho)w_m^{(1)}(\rho)\right] . \tag{3.21}$$

To obtain the final form of the sum rules we shall eliminate the appearance of the first derivative in the term $\langle m|g^{(2)}(\rho)(d/d\rho)m\rangle$. To this end, we go back to (3.16) and choose

$$W(\rho) = g^{(1)}(\rho) . \tag{3.22}$$

Following the same steps as in the previous calculation we find

$$\langle m|g^{(3)}(\rho)m\rangle + 2\left\langle m\left|g^{(2)}(\rho)\frac{d}{d\rho}m\right\rangle = -\lim_{\rho\to 0} g^{(2)}(\rho)|w_m(\rho)|^2 . \tag{3.23}$$

From (3.21) and (3.23) we get finally

$$-\tfrac{1}{2}\langle m|g^{(3)}(\rho)m\rangle - 2e_m\langle m|g^{(1)}(\rho)m\rangle + 2\langle m|g^{(1)}(\rho)U(\rho)m\rangle + \langle m|g(\rho)U^{(1)}(\rho)m\rangle = \lim_{\rho\to 0}\left[\tfrac{1}{2}g^{(2)}(\rho)|w_m(\rho)|^2 + g(\rho)|w_m^{(1)}(\rho)|^2 - g(\rho)w_m^*(\rho)w_m^{(2)}(\rho) - g^{(1)}(\rho)w_m^*(\rho)w_m^{(1)}(\rho)\right] . \tag{3.24}$$

We must stress that up until now the above calculations are *purely formal*. This is because we have not yet placed any constraint whatsoever on the functions $g(\rho)$ when $\rho \to 0$. Therefore it may well be that neither the matrix elements nor the limit of the right-hand side have any finite value. The important point is, however, that as soon as the right-hand side has a finite value, the left-hand side has also a finite value and (3.24) is *indeed the correct relation.*[20]

IV. ILLUSTRATIONS AND APPLICATIONS

This section is entirely devoted to one goal: to show the importance of the information content of the sum rules (3.24). Let us first remind the reader of the boundary conditions on the eigenfunctions $w_{nl}(\rho)$:

$$\text{(a)}\quad w_{nl}(\rho) \underset{\rho\to 0}{\longrightarrow} a_{nl}\rho^{l+1}, \tag{4.1}$$

$$\text{(b)}\quad \lim_{\rho\to\infty} \rho^k |w_m(\rho)| \to 0 \quad \text{for any } k. \tag{4.2}$$

The case $g(\rho)=\rho^\eta$. From (3.21) and (4.1) the boundary term called S has the following expression:

$$S = \frac{(1-\eta)(2l+2-\eta)}{2}|a_{nl}|^2 \lim_{\rho\to 0}(\rho^{2l+\eta}). \tag{4.3}$$

We distinguish two different situations:

(1) $\eta > -2l$. Here

$$S=0 \tag{4.4}$$

and the sum rules (3.24) can be written[23]

$$e_{nl}\langle nl\,|\rho^{\eta-1}|nl\rangle = \langle nl|\rho^{\eta-1}V(\rho)|nl\rangle + \frac{1}{2\eta}\langle nl|\rho^\eta V^{(1)}(\rho)|nl\rangle + \frac{\eta-1}{2\eta}\left[2l(l+1)-\frac{\eta(\eta-2)}{2}\right]\langle nl|\rho^{\eta-3}|nl\rangle . \tag{4.5}$$

In writing this relation, we have used (2.11) to separate the contribution of the centrifugal barrier. This last contribution vanishes if and only if $\eta=1$. For $\eta=1$, using (2.8) and the definition (2.15), we get the well known Clausius relation[17,18]

$$e_{nl} = \langle V(\rho)\rangle_{nl} + \langle \tfrac{1}{2}\rho V^{(1)}(\rho)\rangle_{nl} . \tag{4.6}$$

The relations of Kramers.[24] We take the Coulomb potential

$$\tilde{V}(r) = -e^2/r . \tag{4.7}$$

From (2.12) and choosing

$$\alpha = \mu e^2 , \tag{4.8}$$

we get

$$V(\rho) = -2/\rho . \tag{4.9}$$

Since

$$e_{nl} = -1/n^2 , \tag{4.10}$$

the equation (4.5) gives a relation between the mean values of different powers of the bound-state radius ρ. It is[25]

$$-\tfrac{1}{2}\eta(\eta-1)(\eta-2)\langle\rho^{\eta-3}\rangle + 2(\eta-1)l(l+1)\langle\rho^{\eta-3}\rangle + 2(1-2\eta)\langle\rho^{\eta-2}\rangle = -\frac{2\eta}{n^2}\langle\rho^{\eta-1}\rangle . \tag{4.11}$$

When we substitutue $\eta+1$ into η and rearrange the different terms we find the desired relations,

$$\frac{\eta+1}{n^2}\langle\rho^\eta\rangle = (1+2\eta)\langle\rho^{\eta-1}\rangle - \tfrac{1}{4}\eta[(2l+1)^2-\eta^2]\langle\rho^{\eta-2}\rangle , \tag{4.12}$$

with $\eta \geq 0$.

From the different relations obtained when η is successively taken equal to $0, 1, 2, \ldots$, we can write all mean values $\langle\rho^k\rangle$ with $k=-1, 0, \ldots$, in terms of the quantum numbers n and l. As a third illustration we consider the following case. When

$$l \geq 1 \quad \text{and} \quad \eta = 0 , \tag{4.13}$$

we are led to the relation

$$\langle nl|V^{(1)}(\rho)|nl\rangle = -\left\langle nl\left|\frac{d}{d\rho}\left(\frac{l(l+1)}{\rho^2}\right)\right|nl\right\rangle \tag{4.14}$$

or equivalently to

$$\langle nl|U^{(1)}(\rho)|nl\rangle = 0, \quad l=1, 2, \ldots . \tag{4.14'}$$

We see that relation (3.4) is indeed valid for all waves except the S wave. It illustrates nicely the action of the centrifugal barrier. In the case of the Coulomb potential it leads to the relation ($l \geq 1$)

$$\langle nl|\rho^{-2}|nl\rangle = l(l+1)\langle nl|\rho^{-3}|nl\rangle . \tag{4.15}$$

In the case of a purely linear (confining) potential

$$V(\rho) = 2\lambda\rho , \tag{4.16}$$

it gives

$$\langle nl|\rho^{-3}|nl\rangle = \frac{\lambda}{l(l+1)} . \tag{4.17}$$

As a final illustration we give a relation between matrix elements of ρ and V which is obtained from Clausius's relation and (4.5) with $\eta=2$. It is valid for any $l \geq 0$ that

$$\langle\rho\rangle\langle V\rangle - \langle\rho V\rangle + \tfrac{1}{4}(2\langle\rho\rangle\langle\rho V^{(1)}\rangle - \langle\rho^2 V^{(1)}\rangle) = \frac{l(l+1)}{2}\langle\rho^{-1}\rangle . \tag{4.18}$$

(2) $\eta = -2l$. From (4.3) we see that S is always *finite* and different from zero. It is written as

$$S = (2l+1)^2|a_{nl}|^2 . \tag{4.19}$$

A look at the left-hand side of (3.24) shows that, with the exception of the second term, each term is infinite because the singularity is too strong at

$\rho = 0$. What we show now is that the centrifugal barrier is such that it cancels all infinities in the sum

$$-\tfrac{1}{2}\langle m|g^{(3)}(\rho)m\rangle + 2\langle m|g^{(1)}(\rho)U(\rho)m\rangle + \langle m|g(\rho)U^{(1)}(\rho)|m\rangle . \quad (4.20)$$

To see this, we separate, using (2.11), the centrifugal barrier from $U(\rho)$ and make the usual assumption that $V(\rho)$ is *less* singular than ρ^{-2} at the origin. A simple calculation shows that the singular part has the form

$$[2l(2l+1)(l+1) - 4l^2(l+1) - 2l(l+1)] \times \langle nl|\rho^{-2l-3}|nl\rangle , \quad (4.21)$$

where the coefficient in front of the matrix element is obviously equal to zero. The relation (3.24) expressed explicitly using $g(\rho) = \rho^{-2l}$ and the relation (4.19) leads to the new set of sum rules

$$4le_{nl}\langle nl|\rho^{-2l-1}|nl\rangle - 4l\langle nl|\rho^{-2l-1}V(\rho)|nl\rangle + \langle nl|\rho^{-2l}V^{(1)}(\rho)|nl\rangle = (2l+1)^2|a_{nl}|^2 \quad (4.22)$$

for all $l \geq 0$.

In these sum rules we see that the centrifugal barriers *never contribute explicitly* because they involve $V(\rho)$ and not $U(\rho)$. This has a clear physical significance. The factor ρ^{-2l}, which enters in each matrix element, allows us to probe the region of space, where the centrifugal barrier dominates the behavior of the wave function. It does it in such a way as to allow us "to see" the residual value of the wave function at $\rho = 0$. This residual value is expressed through the boundary term.

These sum rules are also particularly interesting in the study of the quarkonium systems. This is because $|a_{nl}|^2$ is directly related to *experimentally measurable quantities*. Therefore the illustrations we give below are directed to the applications to the quarkonium systems.

The S wave. Here (4.22) reduces to

$$|a_{n0}|^2 = \langle n0|V^{(1)}(\rho)|n0\rangle . \quad (4.23)$$

Written in terms of the usual radial wave function defined in (2.1), it becomes

$$|\tilde{R}_{S_m}(0)|^2 = \alpha^3\langle V^{(1)}(\rho)\rangle_{n0} . \quad (4.24)$$

In terms of $\tilde{V}(r)$ it becomes

$$|\tilde{R}_{S_n}(0)|^2 = 2\mu\langle \tilde{V}^{(1)}(r)\rangle_{n0} . \quad (4.25)$$

This is a well known relation[16] already widely used to study the ψ-like and Υ-like particles.[14]

Before we proceed, we want to make a remark concerning the form (4.24) of the sum rule. It is particularly useful to express the scaling properties, i.e., the relation between different quarkonium spectra. The reason for this is that if scaling holds, $V(\rho)$ must not depend on the reduced mass μ. Therefore the μ dependence of $|\tilde{R}_S(0)|^2$ is entirely contained in the μ dependence of α.[14,26,27] In the particular case of the QCD Coulomb-type potential

$$\tilde{V}(r) = -\frac{4}{3}\frac{\alpha_s}{r} , \quad (4.26)$$

it is convenient to choose

$$\alpha = \tfrac{4}{3}\mu\alpha_s = a^{-1} , \quad (4.27)$$

where a is the "Bohr radius" of quarkonium and (4.24) gives

$$|\tilde{R}_{S_n}(0)|^2 = 2a^{-3}\langle\rho^{-2}\rangle_{n0} . \quad (4.28)$$

If the potential is oscillatorlike and takes the form[28]

$$\tilde{V}(r) = \tfrac{1}{2}\mu\omega_0^2 r^2 , \quad (4.29)$$

we get analogously

$$\alpha = (\mu\omega_0)^{1/2} , \quad V(\rho) = \rho^2 , \quad (4.30)$$

and

$$|R_{S_n}(0)|^2 = 2(\mu\omega_0)^{3/2}\langle\rho\rangle_{n0} . \quad (4.31)$$

Formulas (4.28) and (4.31) display the scaling behavior of $|R_{S_n}(0)|^2$ explicitly.

When the potential includes *several components*, the relation (4.24) can again be written to make the μ dependence explicit. To show this, we take

$$\tilde{V}(r) = -\frac{4}{3}\frac{\alpha_s}{r} + \alpha_c r . \quad (4.32)$$

A simple calculation shows that

$$|\tilde{R}_{n0}(0)|^2 = 2(\alpha_c\mu + a^{-3}\langle\rho^{-2}\rangle_{n0}) . \quad (4.33)$$

The behavior in μ of the first term depends on the assumptions we make on the μ dependence of α_c. If confinement forces are assumed to be *independent of* μ then the first term behaves like μ and the second term like μ^3. However, (4.33) shows clearly that we can easily modify the scaling behavior of $|\tilde{R}_{nS}(0)|^2$ *without changing the functional form of the potential*. The cost is only the introduction of some μ dependence in α_c.

The P wave. Equation (4.22) gives

$$|R^{(1)}_{P_n}(0)|^2 = \tfrac{1}{9}\alpha[\langle\rho^{-2}V^{(1)}\rangle_{n1} + 4e_{n1}\langle\rho^{-3}\rangle_{n1} - 4\langle\rho^{-3}V\rangle_{n1}] , \quad (4.34)$$

or, using (2.7)

$$|\tilde{R}^{(1)}_{P_n}(0)|^2 = \tfrac{1}{9}\alpha^5[\langle\rho^{-2}V^{(1)}\rangle_{n1} - 4\langle\rho^{-3}V\rangle_{n1} + 4e_{n1}\langle\rho^{-3}\rangle_{n1}]\,. \quad (4.35)$$

Contrary to the S-wave formula, this relation contains a dependence on the *energy* of the state. We can eliminate this dependence if we take into account Eq. (4.6), but since e_{n1} is an experimental quantity, it is not necessarily advantageous. On the other hand, we see from (4.6) that e_{n1} is very sensitive to the large-distance behavior of the potential (and of the wave function). This is in contrast to the matrix elements in Eq. (4.35) which are sensitive to the short-distance behavior of the potential and of the wave function. Now $|\tilde{R}^{(1)}_{P_n}(0)|^2$ can be related to the decays of the $^3P_{0,2}Q\bar{Q}$ states into a pair of photons or gluons by the formulas[29]

$$\begin{bmatrix}\Gamma(^3P_0 \to 2\gamma)\\ \Gamma(^3P_2 \to 2\gamma)\end{bmatrix} = \begin{bmatrix}27\alpha^2 e_Q{}^4\\ \frac{36}{5}\alpha^2 e_Q{}^4\end{bmatrix}\frac{|\tilde{R}'_P(0)|^2}{m_Q^4}\,, \quad (4.36)$$

$$\begin{bmatrix}\Gamma(^3P_0 \to 2g)\\ \Gamma(^3P_2 \to 2g)\end{bmatrix} = \begin{bmatrix}6\alpha_s{}^2\\ \frac{8}{5}\alpha_s{}^2\end{bmatrix}\frac{|\tilde{R}'_P(0)|^2}{m_Q^4}\,. \quad (4.36')$$

We do not yet have data on these quantities, but there is reasonable hope of getting them in the near future.

In all cases where we can make $V(\rho)$ independent of the reduced mass of the quarkonium system, we get the scaling formula

$$S_P = \frac{|R^{(1)}_{P,Q'\bar{Q}'}(0)|^2}{|R^{(1)}_{P,Q\bar{Q}}(0)|^2} = \left(\frac{\alpha_{Q'\bar{Q}'}}{\alpha_{Q\bar{Q}}}\right)^5. \quad (4.37)$$

For instance, when

$$\tilde{V}(r) = ar^\epsilon\,, \quad (4.38)$$

we find

$$S_P = \left(\frac{m_{Q'}}{m_Q}\right)^{5/(2+\epsilon)}. \quad (4.39)$$

Taking for α the usual expression[14]

$$\alpha = \left(\frac{\mu}{m_0}\right)^{1/(2+\epsilon)} m_0\,, \quad (4.40)$$

from (4.35) we get

$$|\tilde{R}^{(1)}_{P_n}(0)|^2 = \frac{m_0{}^5}{9}\left(\frac{\mu}{m_0}\right)^{5/(2+\epsilon)}[2\lambda(\epsilon-4)\langle\rho^{\epsilon-3}\rangle_{n1} + 4e_{n1}\langle\rho^{-3}\rangle_{n1}]\,, \quad (4.41)$$

with

$$e_{n1} = 2\lambda(1+\epsilon/2)\langle\rho\rangle_{n1}\,. \quad (4.42)$$

When $\epsilon = 1$, using Eq. (4.17), we obtain

$$|\tilde{R}^{(1)}_{P_n}(0)|^2 = \frac{2\lambda}{9}\left(\frac{\mu}{m_0}\right)^{5/3} m_0{}^5[(2\lambda+1)\langle\rho\rangle_{n1} - 3\langle\rho^{-2}\rangle_{n1}]\,. \quad (4.43)$$

When $\epsilon = -1$, we take instead of (4.40)

$$\alpha = \tfrac{4}{3}\mu\alpha_s = a^{-1}\,, \quad \lambda = -1\,, \quad (4.44)$$

and the corresponding expression is

$$|\tilde{R}^{(1)}_{P_n}(0)|^2 = 2\frac{a^{-5}}{9}[5\langle\rho^{-4}\rangle_{n1} - 2\langle\rho^{-1}\rangle_{n1}\langle\rho^{-3}\rangle_{n1}]\,. \quad (4.45)$$

We can readily calculate it and we obtain

$$|\tilde{R}^{(1)}_{P_n}(0)|^2 = \tfrac{4}{9}a^{-5}\frac{(n^2-1)}{n^5}\,. \quad (4.46)$$

This result is, of course, already known since the Coulomb case is completely solved. For $n=1$ the right-hand side is zero since in that case l is necessarily equal to zero. Therefore, the two gluon decays (4.36) of the P states around 3.5 GeV are *very sensitive* to the *non-Coulombic* part of the potential. Present model calculations[30] show that

$$|\tilde{R}^{(1)}_{P_1}(0)|^2 \simeq 4\times 10^{-2}\ \text{GeV}^5 \quad (4.47)$$

with $m_c = 1.2$ GeV.

The D wave. In this case we get

$$|\tilde{R}^{(2)}_{D_n}(0)|^2 = \tfrac{1}{25}\alpha^9[\langle\rho^{-4}V'\rangle_{n2} - 8\langle\rho^{-5}V\rangle_{n2} + 8e_m\langle\rho^{-5}\rangle_{n2}]\,. \quad (4.48)$$

The discussion for the P wave also applies for the D wave.

Again, the connection with the experimental data is given by the decay widths of the D states. We have[29]

$$\Gamma(^3D_1 \to e^+e^-) = \frac{200\alpha^2 e_Q{}^2}{M_D{}^6}|\tilde{R}''_D(0)|^2\,,$$

$$\Gamma(^1D_2 \to 2g) = \tfrac{2}{3}\alpha_s{}^2\frac{|\tilde{R}''_D(0)|^2}{M_D{}^6}\,.$$

For lack of experimental data we cannot pursue the comparison between the theoretical formula (4.48) and the experiment any further.

V. CONCLUSIONS AND REMARKS

We have shown how hypervirial theorems correctly generalized to include "boundary" effects can lead to interesting sum rules for the radial wave Schrödinger equation. The two simplest ones, i.e., Eqs. (4.6) and (4.24), have already been used in the discussions on quarkonium. This is not the case for all other sum rules. Among

these new sum rules, those which give the expression of the square of the lth derivative of the wave function at the origin are particularly interesting.

The fact that the sum rules (4.5) stress the *long-range part* of the potential and of the wave function, and more so, for increasing values of η, suggests a method of calculation in which the potential is replaced by its confining part and the wave function by its WKB approximation. Such a method would be very analogous to the one used recently by Blankenbecler and Richardson for the one-dimensional oscillator.[31]

Moreover, it is also expected that E_{nl} scales more and more like $\mu^{-1/3}$ when l increases if the confining potential is linear and flavor independent. Again we lack data to verify this fact. The sum rules (4.22) depend more and more on the short-range component of the potential when l increases. Therefore we expect that

$$|\tilde{R}^{(l)}(0)|^2 \tag{5.1}$$

can scale differently from E_{nl} when $l \geq 1$. Again we can hope to check this in the near future.

An approximate calculation of these sum rules can also be performed if we first insert the value of e_{nl} and compute the different matrix elements using only the *short-range part* of the potential.

Sum rules which involve radiative transition matrix elements can also be deduced. An interesting case is

$$\sum_i (e_m - e_i)^2 |\langle m|\rho|i\rangle|^2 = 2\langle m|\rho U^{(1)}(\rho)|m\rangle\,, \tag{5.2}$$

which is obtained from

$$\langle m|[H,\rho][\rho,H]|m\rangle = 0\,. \tag{5.3}$$

If $l=0$ and if

$$V = \frac{4}{3}\frac{\alpha_s}{r} + V_c\,, \tag{5.4}$$

where V_c is the confining potential, using (4.6) and (5.2) we can write

$$\langle V_c\rangle_{n0} + \langle \rho V_c^{(1)}\rangle_{n0} = e_{n0} + \tfrac{3}{4}\sum_i (e_m - e_i)^2 |\langle m|\rho|i\rangle|^2\,. \tag{5.5}$$

This relation expresses V_c entirely in terms of *physically measurable quantities*.

Finally, we want to make a comment on the generalization of the above formulation to include spins. It is well known that we can always make a partial-wave decomposition in terms of the quantum numbers J, L, and S. For the quarkonium systems this decomposition is analogous to that in nucleon-nucleon scattering.[32] The difference is that one obtains four radial wave equations among which two are coupled. Though more involved, the previous sum rules can also be written down.

Note added. After completion of this work we became aware of a paper by C. Quigg and J. L. Rosner [Fermilab Report No. Pub-79/22 (unpublished)] in which our sum rules (4.5) and (4.22) are deduced by direct calculations. The connection of those sum rules to the generalized form of the hypervirial theorems is however overlooked.

Note added in proof. Recently we became aware of a work by A. Khare [Nucl. Phys. B152, 533 (1979)], where the relation (4.22) is also derived.

[1] J. J. Aubert *et al.*, Phys. Rev. Lett. 33, 1404 (1974); J. Augustin *et al.*, *ibid.* 33, 1406 (1974); G. S. Abrams *et al.*, *ibid.* 33, 1453 (1974).

[2] W. Braunschweig *et al.*, Phys. Lett. 57B, 407 (1975); G. J. Feldman *et al.*, Phys. Rev. Lett. 35, 821 (1975); G. J. Feldman and M. L. Perl, Phys. Rep. 33C, 285 (1977).

[3] J. D. Jackson, in *Weak Interactions at High Energy and the Production of New Particles*, proceedings of SLAC Summer Institute on Particle Physics, 1976, edited by M. Zipf (SLAC, Stanford, 1977).

[4] T. Appelquist and H. D. Politzer, Phys. Rev. Lett. 34, 43 (1975); Phys. Rev. D 12, 1404 (1975); B. J. Harrington, S. Y. Park, and A. Yildiz, Phys. Rev. Lett. 34, 168 (1975). E. Eichten *et al.*, *ibid.* 34, 369 (1975); 36, 500 (1976); R. Barbieri, Nucl. Phys. B105, 125 (1976); J. S. Kang and H. J. Schnitzer, Phys. Rev. D 12, 841 (1975).

[5] L. M. Lederman, in *Proceedings of the 1977 European Conference on Particle Physics, Budapest*, edited by L. Jenik and I. Montvay (CRIP, Budapest, 1978). D. M. Kaplan *et al.*, Phys. Rev. Lett. 40, 435 (1978).

[6] E. Eichten and K. Gottfried, Phys. Lett. 66B, 286 (1977).

[7] S. L. Glashow and S. Weinberg, Phys. Rev. D 15, 1958 (1977).

[8] M. Kobayashi and K. Maskawa, Prog. Theor. Phys. 49, 652 (1973); L. Maiani, Phys. Lett. 62B, 183 (1976); F. G. Gilman and M. B. Wise, *ibid.* 83B, 83 (1979).

[9] H. Fritszch, Nucl. Phys. B155, 189 (1979); G. Preparata, Phys. Lett. 82B, 398 (1979); S. Pakvasa and H. Sugawara, *ibid.* 82B, 105 (1979).

[10] T. Kogut and L. Susskind, Phys. Rev. D 9, 2273 (1973); K. G. Wilson, *ibid.* 10, 2445 (1974).

[11] R. L. Jaffe and K. Johnson, Comments Nucl. Part. Phys. 7, 107 (1977).

[12] See for instance L. Susskind, in Les Houches Lectures, 1976 (unpublished); W. Fischer, Nucl. Phys. B129, 157 (1977).

[13] Z. S. Agranowich and V. A. Marchenko, *The Inverse Problem of Scattering Theory* (Gordon and Breach, New York, 1963).

[14] H. B. Thacker, C. Quigg, and J. L. Rosner, Phys. Rev. D 18, 274 (1978); 18, 287 (1978); C. Quigg and

J. L. Rosner, Comments Nucl. Part. Phys. 8, 11 (1978).
[15]H. Grosse and A. Martin, Nucl. Phys. B148, 413 (1978).
[16]M. Fradkin and F. Calogero, Nucl. Phys. 75, 475 (1966).
[17]J. O. Hirshfelder, J. Chem. Phys. 33, 1462 (1960).
[18]A. Martin, Phys. Lett. 67B, 330 (1977).
[19]R. J. Swenson and S. H. Danforth, J. Chem. Phys. 57, 1734 (1972).
[20]A. Burnel and H. Caprasse, Liege Report No. U. Lg. PTM-79/9 (unpublished). In the case of the radial wave equation, ρ and $d/d\rho$ are not canonically conjugate variables.
[21]Analogous statements can be found in several places in the literature. See, for instance, W. Pauli in *Handbuch der Physik*, edited by S. Flügge (Springer, Berlin, Germany, 1958), Vol. V, part I; S. G. Eckstein, B. B. Varga, and S. Aks, Nuovo Cimento 8B, 451 (1972).
[22]An operator G is said to by symmetric if $\langle g|Gf\rangle^* = \langle f|Gg\rangle$ for any f, $g \subset D(G)$, where $D(G)$ is dense in the Hilbert space. The symmetry property is the same as the Hermiticity property. In $D(G)$ the usual Dirac notation gets its full meaning since the expression $\langle g|G|f\rangle$ stresses the fact that we can act with the *same operator* G either on $|f\rangle$ or on $\langle g|$.
[23]Here and subsequently, Dirac notations are reintroduced whenever the operators involved are obviously symmetric.
[24]See, for instance, F. Contantinescu and E. Maggari, *Problems in Quantum Mechanics* (Pergamon, New York, 1976).
[25]We stress that here η is a continuous variable.
[26]H. Caprasse, Lett. Nuovo Cimento 25, 245 (1979).
[27]R. C. Warner and G. C. Joshi, Hadronic J. 2, 198 (1979).
[28]Here the coupling has an explicit μ dependence; consequently, the scaling properties are also different. If more generally $\tilde{V}(r) = ar^\epsilon$ with $a = \lambda\mu^\beta m^{1+\epsilon-\beta}$ and λ *dimensionless and universal*, we get $V(\rho) = 2\lambda\rho$ of $\alpha = (\mu/m)^{(1+\lambda)/(2+\epsilon)} m_0$. See also Ref. 27.
[29]V. A. Novikov, *et al.*, Phys. Rep. 41C, 1 (1978); H. Krasemann, Z. Phys. C1, 189 (1979).
[30]M. Krammer and H. Krasemann, lectures given at the International Universitätwochen für Kernphysik, Schladming, 1979, DESY Report No. 79-20 (unpublished).
[31]J. L. Richardson and R. Blankenbecler, Phys. Rev. D 19, 496 (1979).
[32]See, for instance, M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964), Chap. 7.