local notation. In DeWitt's argument, one then merely has to replace his line-dependent gauge by our "gauge-independent" radiation gauge, which makes the auxiliary quantities a_μ depend merely on the field strengths $F_{\nu\sigma}$ and the Lorentz frame, without introducing any arbitrary elements that would make the potentials become quantities that depend on some other variables than the field strengths alone.

6. CONCLUDING REMARK

I hope that the above has brought out the following. In electrodynamics, one has a free choice between working with potentials or working with field strengths. More precisely, at least three choices are possible: (1) a local, manifestly covariant theory based on a set of operators α which contain physically redundant variables and of which the eigenfunctions Ψ_α do not form an ordinary Hilbert space; (2) a quasi-local theory, which in its field equations hides nonlocal features by the use of abbreviations like a_μ in the radiation gauge or A_μ for DeWitt's line-dependent gauge, but which cannot hide its nonlocality in its quantization; and (3) an openly nonlocal theory, which admits that the potentials are merely abbreviations for certain integrals of the field strengths. Here "nonlocal" refers to field equations for the field variables used, though these variables need not be observables. Choices (2) and (3) avoid nonphysical annexes to Hilbert space and allow the use of actual *observables* as a basic complete set of commuting variables α. The choice between the possibilities (1), (2), and (3), however, is largely a question of *convenience* for whatever use of the theory one has in mind. The idea must be dispelled that the same choice should necessarily be made under all circumstances and for all purposes. The mathematical advantages of the conventional local theory may sometimes outweigh the physical and metaphysical advantages of formulating the theory in the apparently more realistic Hilbert space of gauge-independent quantum electrodynamics.

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Volume Dependence of the Energy of an Enclosed Quantum Mechanical System

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A sum rule is developed that allows one to write a closed form expression for d^2E_n/dV^2; where $E_n(V)$ is the nth eigenvalue and V the volume of an enclosed many-body system with arbitrary interaction potential. This results in a simple differential equation for $E_n(V)$. Unfortunately, the solution, $E_n(V)$, does not appear to be physically meaningful. The reason for this is the appearance of unacceptable functions in the formal development of the sum rule. Because these functions do not belong to the linear manifold with respect to which the Hamiltonian is Hermitian, considerable care must be exercised in applying reduction formulas. Several examples are considered in detail.

I. INTRODUCTION

IN this paper we are concerned with Hermitian operators. Our attention, however, is directed, in particular, to those functions that do not satisfy Eq. (1) below. To begin, consider the following definition[1]: Let Ψ and Φ be *any* two "acceptable" functions defined in a certain region of configuration space τ; an Hermitian operator $\mathbf{O}$, then, has the property that

$$\int_\tau \Psi^*\mathbf{O}\Phi d\tau = \int_\tau \Phi\mathbf{O}^*\Psi^* d\tau. \tag{1}$$

The most crucial part of this definition of an Hermitian operator involves the word "acceptable." The latter usually implies that Ψ and Φ vanish sufficiently strongly on the surface that encloses the region τ of configuration space. The functions Ψ and Φ are also assumed to be quadratically integrable. A very thorough definition of "acceptable" function is given, for example, by Kemble.[2] Thus, his class D functions must, among other things, vanish at infinity faster than any negative power of the coordinates. The latter is also true of the first two derivatives and the functions and their derivatives must also be quadratically integrable.

Of course, less stringent requirements on the wave functions still preserve a Hermitian character. For example, if $\mathbf{O}$ has the form

$$\mathbf{O} \equiv \frac{d}{dx}\left(p(x)\frac{d}{dx}\right) - q(x), \tag{2}$$

and a linear manifold of functions $\Psi_1, \Psi_2, \cdots$ exists such

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[1] H. Margenau and G. M. Murphy, *The Mathematics of Physics of Chemistry* (D. Van Nostrand Company, Inc., Princeton, New Jersey, 1956), 2nd ed., p. 269.

[2] E. C. Kemble, *Quantum Mechanics*, (Dover Publications, New York, 1958), p. 197.

that

$$\mathbf{O}\Psi_1=\lambda_1\Psi_1, \quad \mathbf{O}\Psi_2=\lambda_2\Psi_2,\cdots,$$

then

$$\int_a^b \Psi_1\mathbf{O}\Psi_2 dx=\int_a^b \Psi_2\mathbf{O}\Psi_1 dx, \tag{3}$$

as long as $\Psi_1 p(x)\Psi_2'|_a=\Psi_1 p(x)\Psi_2'|_b$. An operator of the form in Eq. (2) is self-adjoint and Hermitian with respect to all functions $\Psi_1,\Psi_2,\cdots$.

In any particular problem, then, one must be cognizant of the relevant boundary conditions before arbitrarily invoking the Hermitian character of the Hamiltonian. Functions with respect to which Eq. (1) is not satisfied are called "unacceptable."

In Sec. II it is shown that "unacceptable" functions occur in even the most familiar problems in quantum mechanics. A later section is devoted to a discussion of the well-known controversy over the derivation of the virial theorem.[3] The controversy, which prevailed for some years, involved the question of the Hermitian character of the Hamiltonian of an enclosed system. In 1950, Cottrell and Paterson[4] presented a detailed discussion of the reasons for the controversy. One of the reasons is that, although the Hamiltonian is certainly Hermitian in the sense that there exists a linear manifold of functions satisfying Eq. (1), "unacceptable" functions occur in the discussion. Because our results are an extension of the work of Cottrell and Paterson, Secs. II and III are devoted to a brief review of their paper.

In Sec. IV a general sum rule is derived that has several applications in many-body quantum mechanics. Section V is devoted to some of the simpler applications. All the results of Sec. V are easy to verify by other methods.[5] In Sec. VI, having developed a method for dealing with certain sums, we apply the method to a fundamental problem and, although the problem seems to be completely solvable, the results are not physically meaningful. The cause of this is shown to be that coordinate derivatives of many-body wave functions are, in general, unacceptable functions because of the boundary conditions imposed when the system is closed and finite. These functions are unacceptable in the sense that they do not belong to the linear manifold of functions with respect to which the Hamiltonian is Hermitian. Thus, an unrestricted assumption concerning the Hermitian character of the Hamiltonian leads to an invalid sum rule when the system is closed and finite. The sum rule applies without limitation when the system is of infinite extension.

[3] See, for example, M. Born and H. S. Green, Proc. Roy. Soc. (London), A**191**, 168 (1947); H. S. Green *ibid.*, **194**, 244 (1948); J. Chem. Phys., **18**, 1123 (1950).

[4] T. Cottrell and S. Paterson, Phil. Mag. **42**, 341 (1951).

[5] See L. Salem, Phys. Rev. **125**, 1788 (1962), who has recently given a generalization of the sum rule presented here.

II. THE PARTICLE IN A BOX

Consider a particle in a one-dimensional box of length L. The normalized wave functions are $\Psi_n(x,L)=(2/L)^{1/2}\sin(n\pi x/L)$ and the boundary conditions satisfied by the Ψ_n are $\Psi_n(0,L)=\Psi_n(L,L)=0$. Transforming to the unit variable $\xi=x/L$ we have $\Psi_n(\xi,L)=(2/L)^{1/2}\sin n\pi\xi$ so that Ψ_n and all its derivatives with respect to L vanish at $\xi=0$ and 1.

On the other hand, $\partial\Psi_n/\partial\xi=(2/L)^{1/2}n\pi\cos n\pi\xi$, which clearly does not vanish at either end point. Thus, only even derivatives with respect to ξ satisfy the same boundary conditions as $\Psi_n(\xi,L)$ itself. That this affects the results of Eq. (1) with regard to the relevant Hamiltonian is seen in the following example.

Consider the integral in Eq. (4).

$$I_1=\left\langle n\left|H\xi\frac{d}{d\xi}\right|n\right\rangle=2\pi n\int_0^1 \sin n\pi\xi H\xi\cos n\pi\xi d\xi. \tag{4}$$

Now, $H\equiv-(\hbar^2/2m)d^2/dx^2$ so that

$$I_1=-\frac{\hbar^2 n\pi}{mL^2}\int_0^1 \sin n\pi\xi\frac{d^2}{d\xi^2}\xi\cos n\pi\xi d\xi, \tag{5}$$

and it is easily seen that $I_1=3\hbar^2n^2\pi^2/4mL^2$. On the other hand,

$$I_2=\langle n|\,\xi(d/d\xi)H\,|n\rangle=-\hbar^2n^2\pi^2/4mL^2. \tag{6}$$

Thus, a necessary condition that the functions involved be acceptable, namely, that the diagonal element of the commutator of the Hamiltonian with the operator that generates the function vanish, is not satisfied. That is,

$$I_1-I_2=\langle n|\,[H,\xi(d/d\xi)]\,|n\rangle=\hbar^2n^2\pi^2/mL^2. \tag{7}$$

Hence, in this simple example, the function $\xi d\Psi_n/\partial\xi$ is "unacceptable."

We note further, since the eigenvalues of this problem are given by $E_n=\hbar^2n^2\pi^2/2mL^2$, that

$$L(dE_n/dL)=-\hbar^2n^2\pi^2/mL^2=\langle n|\,[\xi(\partial/\partial\xi),H]\,|n\rangle, \tag{8}$$

a result that will prove of interest in our discussion of the virial theorem. Thus, in the following section it is shown, in agreement with Eq. (8), that the term LdE_n/dL is a measure of the "unacceptability" of the function $\mathbf{r}\cdot\nabla\Psi_n$, even in the general many-particle problem.

III. THE GENERAL CASE

Consider a system of N particles described by a Hamiltonian, $H=T+U$. Let the system be enclosed in a volume $V=L^3$. We accordingly define the reduced vectors $\boldsymbol{\xi}_i=\mathbf{x}_i/L$ and impose upon the eigenfunctions Ψ_n the standard boundary condition that Ψ_n vanish for any vector on the surface.

If we now assume that H is Hermitian and all func-

tions involved are acceptable, it follows that[6]

$$\langle n|[\mathbf{x}_i\partial/\partial\mathbf{x}_i,H]|n\rangle=\langle n|[\xi_i d/\partial\xi_i,H]|n\rangle=0, \quad (9)$$

where the average, $\langle\rangle$, is over the unit cube (i.e., every coordinate ξ_{ij} varies from zero to 1).

It is evident,[6] if the commutator bracket in Eq. (9) is expanded, that

$$2\langle n|\mathbf{p}_i\cdot\mathbf{p}_i/2m_i|n\rangle=\langle n|\xi_i\partial U/\partial\xi_i|n\rangle, \quad (10)$$

where the quantities in Eq. (10) have their usual significance. Summing over all particles Eq. (10) becomes

$$2\langle n|T|n\rangle=\langle n|\sum_i\xi_i\partial U/\partial\xi_i|n\rangle. \quad (11)$$

On the other hand, it is well known[4] that a system enclosed in a finite volume satisfies the virial theorem

$$L(dE_n/dL)+2\langle n|T|n\rangle=\langle n|\sum_i\xi_i\partial U/\partial\xi_i|n\rangle, \quad (12)$$

and, thus, Eq. (11) can only be valid in the limit as $L\rightarrow\infty$. But our derivation was presumably valid for all values of L!

This apparent paradox is easily resolved when it is recalled that the only assumption that led to Eq. (11) was that the linear manifold of H included *all* of the functions involved in Eq. (9). It is clear then that this assumption is not valid and, just as in the simple particle-in-a-box, $\xi_i\partial|n\rangle/\partial\xi_i$ is "unacceptable." As a matter of fact, just as in Sec. II, we must have

$$L(dE_n/dL)=\langle n|[\sum_i\xi_i\partial/\partial\xi_i,H]|n\rangle, \quad (13)$$

in order to make Eqs. (11) and (12) consistent. Equation (13) can also be put in terms of the eigenpressure P_n since $LdE_n/dL=-3VP_n$. Thus, we have the result that

$$P_nV=\tfrac{1}{3}\langle n|[H,\sum_i\xi_i\partial/\partial\xi_i]|n\rangle, \quad (14)$$

or, that the eigenpressure-volume product is a measure of the "unacceptability" of $\xi_i\partial|n\rangle/\partial\xi_i$. The previous results are significant in the sense that they demonstrate that both sides of the "virial theorem controversy" were correct. That is, the Hamiltonian is certainly Hermitian with respect to a linear manifold of functions of which parameter derivatives are included, although Eq. (1) is not satisfied with respect to functions involving coordinate derivatives.

Before proceeding, it is of some interest to note that if a statistical average is performed on Eq. (14) the result is the thermodynamic PV product—a quantity that is related to the temperature of the system. We might conclude then that it is fortunate that the functions $\xi_i\partial|n\rangle/\partial\xi_i$ are "unacceptable," otherwise there would be no basis for a definition of the ideal gas temperature. This result has a simple physical interpretation. Thus, since $\partial|n\rangle/\partial\xi_i$ is essentially the instantaneous momentum of the ith particle, physically one would expect that its value on the wall, when statistically averaged, would be a measure of the temperature of the system. It appears then that Eq. (14) allows for some physical insight into a quantum-statistical definition of temperature, for if $\partial|n\rangle/\partial\xi_i$ did vanish on the wall, it would be an acceptable function and the right-hand side of Eq. (14) would also vanish. It appears then that it is a physical necessity that $\partial|n\rangle/\partial\xi_i$ be nonvanishing on the wall of the enclosure.

[6] W. L. Clinton, J. Chem. Phys., **33**, 1603 (1960).

IV. GENERAL SUM RULE

There are many theorems in classical mechanics that find immediate use when carried over to quantum mechanics. Although, as we will show later, the sum rule we will be concerned with can be derived more directly, it will be instructive to show how an equation from classical mechanics can lead one to useful results.

An equation in classical mechanics due to Jacobi[7] reads

$$d^2J/dt^2=2T+u, \quad (15)$$

where $J=1/2\sum_i m_ir_i^2$ is Jacobi's function, u is an inverse r_{ij} type potential, T is the kinetic energy of the system, and t is the time. In quantum mechanics the second time derivative is replaced by a double commutator so that Eq. (15) becomes

$$-[H,[H,J]]=2T+u, \quad (16)$$

or, in terms of a representation $|n\rangle,|m\rangle,\cdots$ in which H is diagonal,

$$-(E_n-E_m)^2\langle n|J|m\rangle=\langle n|T|m\rangle;\ n\neq m, \quad (17)$$

since

$$\langle n|H|m\rangle=\langle n|T|m\rangle+\langle n|u|m\rangle=0 \text{ for } n\neq m.$$

It is clear now that any perturbation type sum-over-states involving $\langle n|T|m\rangle$ can be put in closed form using the transformation (17). Thus for a sum of the form

$$S_n=\sum_{m\neq n}\frac{\langle n|T|m\rangle\langle m|O|n\rangle}{E_n-E_m}, \quad (18)$$

we have, using (17)

$$S_n=-\sum_{m\neq n}\langle n|[H,J]|m\rangle\langle m|O|n\rangle=\langle n|[H,J]O|n\rangle, \quad (19)$$

where O is an arbitrary operator[8] and $\langle n|[H,J]|n\rangle=0$.

Since the Jacobi equation applies only to inverse r_{ij} potentials, the preceding lacks generality. It will, therefore, be advantageous to present a more general and, at the same time, more elegant proof of the sum rule.

Consider then, a system of N particles having position and momenta vectors $\mathbf{r}_1,\cdots\mathbf{r}_N$ and $\mathbf{p}_1,\cdots\mathbf{p}_N$ and being described by the Hamiltonian $H=T+u$. We

[7] E. T. Whittaker, *Analytical Dynamics* (Cambridge University Press, New York, 1927), p. 342.

[8] See later discussion of "unacceptable functions" with regard to the arbitrariness of the operator O.

write the commutator of $\mathbf{r}_k\cdot\nabla_k$ with H as

$$[\mathbf{r}_k\cdot\nabla_k,H]=[\mathbf{r}_k,H]\cdot\nabla_k+\mathbf{r}_k[\nabla_k,H], \tag{20}$$

from which it follows that

$$[\mathbf{r}_k\cdot\nabla_k,H]=-(\mathbf{p}_k\cdot\mathbf{p}_k/m_k)+\mathbf{r}_k\cdot(\nabla_k u). \tag{21}$$

Summing over all particles and using the fact that $H|n\rangle=E_n|n\rangle$ we have

$$(E_m-E_n)\langle n|\sum_k\mathbf{r}_k\cdot\nabla_k|m\rangle=-2\langle n|T|m\rangle+\langle n|\mathcal{U}|m\rangle, \tag{22}$$

where $\mathcal{U}\equiv\sum_k\mathbf{r}_k\cdot(\nabla_k u)$. It is apparent then that any sum of the type

$$S_n=\sum_{m\neq n}\frac{\langle n|2T-\mathcal{U}|m\rangle\langle m|O|n\rangle}{E_n-E_m} \tag{23}$$

is immediately reducible using the transformation (22). Thus

$$S_n=\sum_{m\neq n}\langle n|\sum_k\mathbf{r}_k\cdot\nabla_k|m\rangle\langle m|O|n\rangle=\langle n|\sum_k\mathbf{r}_k\cdot\nabla_k O|n\rangle-\langle n|\sum\mathbf{r}_k\cdot\nabla_k|n\rangle\langle n|O|n\rangle. \tag{24}$$

Of course, in the event that u is a homogeneous function of the coordinates, of degree σ, then $2T-\mathcal{U}=2T-\sigma u$ and

$$\langle n|2T-\mathcal{U}|m\rangle=(2+\sigma)\langle n|T|m\rangle, \tag{25}$$

since

$$\langle n|T|m\rangle=-\langle n|u|m\rangle \text{ for } n\neq m.$$

V. PARAMETER DEPENDENCE OF EIGENVALUE AND EIGENFUNCTION

In general, it is necessary to reduce infinite sums in order to determine variations in Ψ with respect to a parameter λ, appearing in the Hamiltonian. Thus, for the nth quantum state, the function $\partial\Psi_n/\partial\lambda$ can be expanded in the complete set $\Psi_1\cdots\Psi_m\cdots$ and

$$\partial\Psi_n/\partial\lambda=\sum_{m\neq n}C_{nm}(\lambda)\Psi_m. \tag{26}$$

The coefficients are easily seen to be

$$C_{nm}(\lambda)=\frac{\langle m|\partial H/\partial\lambda|n\rangle}{E_n-E_m}, \tag{27}$$

since $H|n\rangle=E_n|n\rangle$. The variation of E_n with respect to λ is easier to ascertain since $dE_n/d\lambda$ does not depend upon $\partial\Psi_n/\partial\lambda$. Thus, as is well known,

$$dE_n/d\lambda=\langle n|\partial H/\partial\lambda|n\rangle. \tag{28}$$

In the event λ can be associated with the kinetic energy, T, alone, Eq. (24) can be applied to reduce any infinite sum. However, in such cases it appears that $E_n(\lambda)$ is always completely determined by Eq. (28). For example, with a system of particles of mass M we can let $M=\lambda$ and $\partial H/\partial\lambda=\partial H/\partial M=-M^{-1}T$ and $dE_n/dM=-M^{-1}\langle n|T|n\rangle$ which is a well-known result.

TABLE I. Mass dependence of the eigenvalue.

Potential	σ	Mass dependence of E_n
Coulomb	-1	M
Harmonic oscillator	2	$M^{-1/2}$
Quartic	4	$M^{-2/3}$
Square well	∞	M^{-1}

One can then apply this to potentials that are homogeneous and of degree σ in the coordinates and because

$$2\langle n|T|n\rangle=\sigma\langle n|u|n\rangle, \tag{29a}$$

$$\langle n|T|n\rangle=E_n-\langle n|u|n\rangle, \tag{29b}$$

we must have that

$$M(dE_n/dM)+[\sigma/(2+\sigma)]E_n=0. \tag{30}$$

The differential equation (30) requires that $E_n=AM^{-(\sigma/2+\sigma)}$, where A may be a function of quantum numbers and other parameters of the system. Table I lists several common potentials to which this can be applied.

Actually, whenever the potential $u(r_1\cdots r_N)$ can be written as $Kf(r_1\cdots r_N)$, the functional form of the energy is easily shown to be

$$E_n=A(\hbar^2/M)^{\sigma/(2+\sigma)}K^{2/(2+\sigma)}. \tag{31}$$

Thus, for example, the harmonic oscillator energy levels must be proportional to $h(K/M)^{1/2}=\hbar\omega$. One could now use our sum rule to obtain a closed form expression for $\partial\Psi_n/\partial\lambda$. However, as also in the case of the energy, dimensionality arguments lead more simply to the same end result.

VI. VOLUME DEPENDENCE OF THE ENERGY OF AN ENCLOSED SYSTEM

Recently Brown[9] has given an expression for the second order adiabatic energy derivative with respect to the volume of an enclosed system of arbitrarily interacting particles. In particular, he has shown that

$$L^2\frac{d^2E_n}{dL^2}=6\langle n|T|n\rangle+\langle n|\sum_K\mathbf{r}_K\cdot(\nabla_K\mathcal{U})|n\rangle-\langle n|\mathcal{U}|n\rangle+2\sum_{m\neq n}\frac{|\langle n|2T-\mathcal{U}|m\rangle|^2}{E_n-E_m}, \tag{32}$$

where L is the cube root of the volume of the enclosure and again $\mathcal{U}$ is the virial function.

Before using our sum rule on (32) we note again that in the derivation of Eq. (22), upon which our reduction is based, it was implicitly assumed that all functions involved belonged to the linear manifold of functions with respect to which the Hamiltonian is Hermitian.

[9] W. B. Brown, Proc. Cambridge Phil. Soc. **58**, 251 (1958).

Thus, insofar as the latter is a valid assumption, the sum in Eq. (32) should easily reduce to one term as shown in Eq. (24). Actually, however, we will show that the resulting expression for d^2E_n/dL^2 leads to a physically untenable conclusion so that our assumption concerning the properties of the functions involved must not be true. Now, the results of Secs. II and III clearly indicate that functions such as $\mathbf{r}_k\cdot\nabla_k\Psi$ do not belong to the proper linear manifold when the system is closed and must, therefore, be termed unacceptable. The following argument, in which our sum rule is paramount, will serve as an additional example.

Substituting Eq. (22) into Eq. (32) we have

$$L^2\frac{d^2E_n}{dL^2}=6\langle n|T|n\rangle+\langle n|\sum_K \mathbf{r}_K\cdot\nabla_K\mathcal{U}|n\rangle-\langle n|\mathcal{U}|n\rangle$$
$$+2\sum_{m\neq n}\langle n|\sum_K \mathbf{r}_K\cdot\nabla_K|m\rangle\langle m|2T-\mathcal{U}|n\rangle. \quad (33)$$

We now take the position that T is Hermitian and ∇_k anti-Hermitian with respect to all $|n\rangle$ and $|m\rangle$. Since $|n\rangle$ and $|m\rangle$ satisfy the same boundary conditions, this is surely correct. Thus, the sum over states, which we will denote by S_n, in Eq. (33) can be written in the following two ways:

$$S_n=\sum_{m\neq n}\langle n|\sum_k \mathbf{r}_k\cdot\nabla_k|m\rangle\langle m|2T-\mathcal{U}|n\rangle, \quad (34a)$$

$$S_n=-\sum_{m\neq n}\langle n|2T-\mathcal{U}|m\rangle\langle m|\sum_k \mathbf{r}_k\cdot\nabla_k|n\rangle. \quad (34b)$$

Upon adding (34a) and (34b) we see that

$$S_n=\tfrac{1}{2}\langle n|[\sum_k \mathbf{r}_k\cdot\nabla_k,\ (2T-\mathcal{U})]|n\rangle, \quad (35)$$

which can easily be shown to reduce to

$$S_n=-2\langle n|T|n\rangle-\tfrac{1}{2}\langle n|\sum_k \mathbf{r}_k\cdot\nabla_k\mathcal{U}|n\rangle. \quad (36)$$

Substituting S_n into Eq. (33) yields

$$L^2d^2E_n/dL^2=2\langle n|T/n\rangle-\langle n|\mathcal{U}|n\rangle. \quad (37)$$

But we know that $-2\langle n|T|n\rangle+\langle n|\mathcal{U}|n\rangle=LdE_n/dL$ so that Eq. (37) becomes

$$L^2d^2E_n/dL^2+LdE_n/dL=0. \quad (38)$$

Now, the solution of Eq. (38) is simple and has the form

$$E_n(L)=A(n)+B(n)\ \ln L \quad (39)$$

for every quantum state.

It is evident on physical grounds that Eq. (39) cannot be correct for it states that, even though A and B may be functions of the quantum state n, the complete volume dependence of *any* eigenstate of *any* many-particle system is given by $E_n=A+\frac{1}{3}B\ \ln V$.

We can only conclude that our use of the sum rule is not valid and the only reason for this appears to be the "unacceptability" of the functions involved. Thus, Eq. (22) is no longer valid since

$$\langle n|[H,\mathbf{r}_k\cdot\nabla_k]|m\rangle\neq(E_n-Em)\langle n|\mathbf{r}_k\cdot\nabla_k|m\rangle,$$

unless the functions $\mathbf{r}_k\cdot\nabla_k|m\rangle$ belong to the proper linear manifold.

VII. FINAL REMARK

We can proceed in another way, however. Suppose we define a matrix element, $\langle n|f|m\rangle$, which when added to the left-hand size of Eq. (22) causes it to be satisfied. This matrix element will be a measure of the extent to which $\mathbf{r}_k\nabla_k\cdot|m\rangle$ is "unacceptable." Eq. (38) will then become

$$L^2d^2E_n/dL^2+LdE_n/dL=F_n(L), \quad (40)$$

where $F_n(L)$ still involves an infinite sum. Certainly $F_n(L)$ is a function of L but the solution of Eq. (40) is easily written down in terms of an integration. Thus, since the solution of the homogeneous part of (40) is $E_n=A+B\ \ln L$ we have

$$E_n(L)=A'(n)+B'(n)\ \ln L$$
$$+\ln L\int F_n(L)LdL-\int F_n(L)L\ \ln L dL. \quad (41)$$

Suppose further that for large volumes, $F_n(L)$ admits of a power series expansion in powers of $1/L$. It is clear then that E_n will be expressible in terms of a series involving functions of the form $(L^K\ \ln L)$ and other logarithmic terms. This approach is presently being investigated.