

Spectral decompositions of certain functionals for the evaluation of quantum-mechanical sums

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1969 J. Phys. A: Gen. Phys. 2 413

(<http://iopscience.iop.org/0022-3689/2/3/022>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 31/05/2010 at 19:37

Please note that [terms and conditions apply](#).

Spectral decompositions of certain functionals for the evaluation of quantum-mechanical sums

Abstract. This letter presents spectral decompositions (in the Dirac formalism) of certain functionals which are useful in finding approximate estimates, through the calculation of rigorous lower and upper bounds to the true value, of some quantum-mechanical sums.

This letter achieves a substantial generalization of some earlier results of the present author (Sharma 1967, 1969, to be referred to as I and II, respectively). The generalized results can be used in the evaluation of some so-called quantum-mechanical sums. The elegance of the method used in this letter derives from its astounding simplicity and the derivations are so straightforward that it is adequate to state merely the crucial results in their final form. In any case the details of the derivations are exactly similar to those described in I and II.

Formalities. We shall denote complex conjugation by an asterisk and Hermitian conjugation by an obelisk. Letters denoting operators will each carry a circumflex. Suppose that in a Hilbert space \mathcal{E} a Hermitian operator \hat{H}_0 has a complete set, in the Dirac (1958) sense, of orthonormal eigenkets $\{|\Phi_n^{(0)}\rangle\}$ belonging to a set of non-degenerate eigenvalues $\{\epsilon_n^{(0)}\}$; the labelling index is so chosen that the eigenvalues form a monotonically increasing sequence and the lowest eigenvalue and the corresponding eigenket are labelled by $i = 0$. It is further supposed that the lowest part of the eigenvalue spectrum of \hat{H}_0 is discrete and the remainder is continuous. Suppose further that \hat{H}_1 is an operator which *may or may not* be Hermitian; we denote the number (in general complex) $\langle \Phi_i^{(0)} | \hat{H}_1 | \Phi_i^{(0)} \rangle$ by $\epsilon_i^{(1)}$. We wish to find the spectral decompositions of functionals whose extrema correspond to the value of the sum $S_{i,r,s}$ given by

$$S_{i,r,s} = -\sum_n' (\epsilon_n^{(0)} - \epsilon_i^{(0)} + \alpha)^r \{(\epsilon_n^{(0)} - \epsilon_i^{(0)} + \alpha)^2 + \beta^2\}^s |\langle \Phi_n^{(0)} | \hat{H}_1 | \Phi_i^{(0)} \rangle|^2 \quad (1)$$

where \sum_n denotes a summation over the discrete spectrum and an integration over the continuous spectrum, and the prime over it denotes that the summation over $n = i$ is omitted, r and s are integers (positive, negative or zero) and α and β are real numbers. For the sake of brevity we introduce the following notations:

$$\hat{g} = \hat{H}_0 - \epsilon_i^{(0)} + \alpha \quad (2)$$

$$\hat{G} = (\hat{H}_0 - \epsilon_i^{(0)} + \alpha)^2 + \beta^2 \quad (3)$$

$$\omega_{ni} = \epsilon_n^{(0)} - \epsilon_i^{(0)} + \alpha \quad (4)$$

$$\Omega_{ni} = (\epsilon_n^{(0)} - \epsilon_i^{(0)} + \alpha)^2 + \beta^2 \quad (5)$$

$$H_{ni} = \langle \Phi_n^{(0)} | \hat{H}_1 | \Phi_i^{(0)} \rangle \quad (6)$$

$$r' = \frac{1}{2}(|r| + r) \quad (7)$$

$$r'' = \frac{1}{2}(|r| - r) \quad (8)$$

and s' and s'' are defined by equations analogous to (7) and (8), respectively. We denote an arbitrary ket by $|\Psi\rangle$ and denote its spectral decomposition by

$$|\Psi\rangle = \sum_n a_n |\Phi_n^{(0)}\rangle. \quad (9)$$

The functionals and their spectral decompositions. The functionals are obtained by modifying those of I and II to fit the requirements of the present problem. We derive them

in such a way that it is unnecessary to restrict $|\Psi^r\rangle$ to the orthogonal complement of the one-dimensional linear manifold spanned by $|\Phi_i^{(0)}\rangle$. For the generalized Hylleraas functional we have

$$\begin{aligned} E_{i,r,s}(|\Psi^r\rangle) &= \langle \Psi^r | \hat{g}^{r|s} \hat{G}^{s|} | \Psi^r \rangle - \alpha^{r|} (\alpha^2 + \beta^2)^{|s|} | \langle \Phi_i^{(0)} | \Psi^r \rangle |^2 \\ &\quad + \langle \Psi^r | \hat{g}^{r'} \hat{G}^{s'} (\hat{H}_1 - \epsilon_i^{(1)}) | \Phi_i^{(0)} \rangle + \langle \Phi_i^{(0)} | (\hat{H}_1^\dagger - \epsilon_i^{(1)*}) \hat{g}^{r'} \hat{G}^{s'} | \Psi^r \rangle \\ &= S_{i,r,s} + \sum_n' \omega_{ni}^{r|} \Omega_{ni}^{s|} \left| a_n + \frac{H_{ni}}{\omega_{ni}^{r''} \Omega_{ni}^{s''}} \right|^2. \end{aligned} \quad (10)$$

Similarly, $|\gamma(|\Psi^r\rangle)\rangle$ of II is now modified to read

$$|\gamma(|\Psi^r\rangle)\rangle = \hat{g}^{r''} \hat{G}^{s''} | \Psi^r \rangle - \alpha^{r''} (\alpha^2 + \beta^2)^{s''} \langle \Phi_i^{(0)} | \Psi^r \rangle | \Phi_i^{(0)} \rangle + (\hat{H}_1 - \epsilon_i^{(1)}) | \Phi_i^{(0)} \rangle. \quad (11)$$

It is convenient to define a functional $F_{i,r,s}$ as follows:

$$\begin{aligned} F_{i,r,s}(|\Psi^r\rangle) &= \langle \gamma | \hat{g}^{r'} \hat{G}^{s'} | \gamma \rangle \\ &= \sum_n' \omega_{ni}^{(r'+2r'')} \Omega_{ni}^{(s'+2s'')} \left| a_n + \frac{H_{ni}}{\omega_{ni}^{r''} \Omega_{ni}^{s''}} \right|^2. \end{aligned} \quad (12)$$

Lower and upper bounds. Suppose N is the smallest integer such that $N \neq i$, and for any integer $t \geq N$

$$\omega_{ti}^{r|} > 0; \quad (13)$$

(when such an integer does not exist the method is still formally valid if relation (13) is true for some continuum index ν , but in such cases the method is not likely to have any practical application) we then have the following bounds for $S_{i,r,s}$:

$$\begin{aligned} E_{i,r,s} - \frac{F_{i,r,s}}{\omega_{Ni}^{r''} \Omega_{Ni}^{s''}} + \sum_{\substack{n < N; \\ n \neq i}} \left\{ \frac{\omega_{ni}^{(r'+2r'')} \Omega_{ni}^{(s'+2s'')}}{\omega_{Ni}^{r''} \Omega_{Ni}^{s''}} - \omega_{ni}^{r|} \Omega_{ni}^{s|} \right\} \\ \times \left| \langle \Phi_n^{(0)} | \Psi^r \rangle + \frac{H_{ni}}{\omega_{ni}^{r''} \Omega_{ni}^{s''}} \right|^2 \leq S_{i,r,s} \\ \leq E_{i,r,s} - \sum_{\substack{n < N; \\ n \neq i}} \omega_{ni}^{r|} \Omega_{ni}^{s|} \left| \langle \Phi_n^{(0)} | \Psi^r \rangle + \frac{H_{ni}}{\omega_{ni}^{r''} \Omega_{ni}^{s''}} \right|^2. \end{aligned} \quad (14)$$

It is to be noted that the subtraction of the summation in the upper bound of relation (14) is *necessary* for establishing a rigorous upper bound and the calculation of the same terms, as in II, allows us to *improve* the lower bound. It is possible to improve the bounds further by progressively extending the summation to values of n higher than N . We also note that a further generalization of these results to the case where the multiplying factor of $|H_{ni}|^2$ in the sum is a ratio of any two polynomials in $\epsilon_n^{(0)}$ with real coefficients is a *mere triviality*.

The spectral decompositions also help us to find better lower bounds than those of relation (14) in particular cases: for example, if $r > 0$, $s = -r$, it is easy to verify that

$$\begin{aligned} E_{i,r,-r} - \frac{\| |\gamma(|\Psi^r\rangle)\rangle \|^2}{\Omega_{Ni}^{r/2}} + \sum_{\substack{n < N; \\ n \neq i}} \left\{ \frac{\Omega_{ni}^{2r}}{\Omega_{Ni}^{r/2}} - \omega_{ni}^r \Omega_{ni}^r \right\} \\ \times \left| \langle \Phi_n^{(0)} | \Psi^r \rangle + \frac{H_{ni}}{\Omega_{ni}^r} \right|^2 \leq S_{i,r,-r}. \end{aligned} \quad (15)$$

Comparison of the error terms in the lower bounds of the inequalities (14) and (15) for this particular case indicates that the latter lower bound is likely to be better than the former for small values of β .

These results not only include all the results derived earlier in I and II and also those derived by a number of other authors (see, for example, Robinson 1969a, b where further references will be found) as particular cases but go very much farther.

Department of Mathematics,
Birkbeck College,
University of London.

C. S. SHARMA
3rd February 1969

DIRAC, P. A. M., 1958, *The Principles of Quantum Mechanics*, 4th edn (Oxford: Clarendon Press).

ROBINSON, P. D., 1969a, *J. Phys. A (Gen. Phys.)*, [2], 2, 193-9.

— 1969b, *J. Phys. A (Gen. Phys.)*, [2], 2, 295-303.

SHARMA, C. S., 1967, *Proc. Phys. Soc.*, 91, 50-3.

— 1969, *J. Phys. A (Gen. Phys.)*, [2], 2, 140-1.

J. PHYS. A (GEN. PHYS.), 1969, SER. 2, VOL. 2. PRINTED IN GREAT BRITAIN

A simple method for calculation of conditions behind shock waves

Abstract. Conditions behind the incident and reflected shock wave in a shock tube are calculated from the initial conditions of pressure, density and temperature, together with the known speed of the incident shock wave. In this method the enthalpy of the gas is regarded as consisting of two parts: (i) the enthalpy evaluated for a gas consisting of molecules having no internal excitation and (ii) a correction term to be added to (i) to take account of internal excitation. An iterative solution to the flow equations for incident and reflected shock waves based on this correction term is obtained. Results for carbon monoxide are given in graphical form.

In shock-tube research the need arises for calculating conditions in shock-heated gases from known initial conditions and the measured shock speed. Although tables are available for some gases, interpolation using a table is not always accurate enough. The method presented here is very well suited for computer use.

In a frame of reference in which the incident shock wave is at rest the equations of state, continuity, momentum and energy are, respectively,

$$p = \rho RT \quad (1)$$

$$\rho_2 u_2 = \rho_1 u_1 = m \quad (2)$$

$$p_2 + \rho_2 u_2^2 = p_1 + \rho_1 u_1^2 = i \quad (3)$$

$$h_2 + \frac{1}{2} u_2^2 = h_1 + \frac{1}{2} u_1^2 = h_0 \quad (4)$$

where h is given by

$$h = (1 + \frac{1}{2}n)RT + \phi(T). \quad (5)$$

p , ρ and T have their usual meanings, R is the gas constant per gramme, u is the flow speed and h is the specific enthalpy. Suffixes 1 and 2 refer to conditions upstream and downstream of the shock wave, respectively. Conditions 1 are assumed known. Clearly, u_1 is the speed of the shock wave in laboratory coordinates. n is the number of degrees of freedom for rigid molecules ($n = 3, 5$ or 6 according as to whether the gas particles are monatomic, linear molecules or non-linear molecules).

Equation (5) shows the enthalpy as consisting of two parts: (i) $(1 + \frac{1}{2}n)RT$, which is the enthalpy appropriate to rigid molecules, and (ii) the term $\phi(T)$, which represents the