International Journal of Science and Research (IJSR)
ISSN: 2319-7064
SJIF (2020): 7.803

On the Extensions of Virial and Feynman - Hellman Theorem

Pratyusha Biswas Deb[1], S. Brajamani (Deceased)[2], H.C. Mohanto[3], Soumya Das[4], P. S. Majumdar[5]

[1]Assistant Professor, Dept of Electrical Engineering, Narula Institute of Technology, West Bengal-700109, India
[2]Professor, Dept of Physics, Manipur University, 795003
[3]Associate Professor, Dept of Mathematics, A.P.C College, New Barrackpore, Kolkata-700131, India
[4]Project Manager, S. M. Technologies Infra Pvt ltd, Kolkara-700001, India
[5]Associate Professor, Dept of Physics, A.P.C College, New Barrackpore, Kolkata-700131, India

Abstract: ***In the present work off diagonal and higher order extensions of Feynman-Hellman theorem is studied Rayleigh-Schrödinger perturbation theory for the degenerate case is redefined using a new technique. We also consider off-diagonal extension of quantum mechanical virial theorem by considering the case of linear harmonic oscillator.***

Keywords: Rayleigh-Schrödinger perturbation theory, Feynman-Hellman theorem, quantum mechanical virial theorem, linear harmonic oscillator

1.Introduction

The Feynman [1] and independently Hellman [2] derived a result known as Feynman-Hellman theorem [FHT]. FHT has been successfully used to calculate expectation values in a number of quantum mechanical system [3, 4].

Epstein [5] obtained Rayleigh- Schrödinger (RS) perturbation theory both non-degenerate and degenerate as a consequence of FHT. He also carried out the off diagonal generalization of Viral theorem [6]. In the present work we consider these extensions of FHT, non-degenerate perturbation theory in FH approach and finally we take up the virial theorems and its generalization.

2.Indentations and Equations

Let us assume that the Hamiltonian of a dynamical system depends on a continuously variable real parameter λ. Its eigenvalues and Eigen functions are then generally functions of λ. Denoting the eigenvalues by $€_i(\lambda)$ and the normalized Eigen functions by $\Psi_i(\lambda)$, we have

$$\{ \Psi_j(\lambda) \mid H(\lambda) \mid \Psi_i(\lambda) \} = €_i(\lambda)\, \delta_{ji} \qquad (1)$$

Differentiating both sides of eqn (1) with respect to λ and assuming validity of differentiation under the integral on the left-hand side we have

$$\{\Psi_j(\lambda)|\frac{\partial H(\lambda)}{\partial\lambda}| \Psi_i(\lambda)\} + [€_j(\lambda) - €_i(\lambda)]\, \alpha_{ji}(\lambda) = \frac{\partial €i(\lambda)}{\partial\lambda}\delta_{ji} \qquad (2)$$

Where the coefficients $\alpha_{ji}(\lambda)$ are defined as

$$\alpha_{ji}(\lambda) = \{ \Psi_j(\lambda)|\frac{\partial H(\lambda)}{\partial\lambda} \} \qquad (3)$$

and satisfy the anti- Hermiticity condition

$$\alpha ij^*(\lambda) = -\alpha ji(\lambda), \text{ for all i and j} \qquad (4)$$

Condition (4) follows upon differentiating with respect to λ and using the orthogonality relations of the Eigen functions

$$\{\Psi j(\lambda)|\frac{\partial H}{\partial\lambda}| \Psi i(\lambda)\} = \frac{\partial €i(\lambda)}{\partial\lambda} \qquad (5)$$

Which is obtained as a special case of Eq. (2) when j = i

Here after, we shall suppress the explicit it indication of λ as an argument of the function unless otherwise demanded. Differentiating eqn (5) with respect to λ we find,

$$\{ \frac{\partial\Psi j}{\partial\lambda}| \frac{\partial H}{\partial\lambda}| \Psi i(\lambda) \} + \{ \Psi j \mid \frac{\partial H}{\partial\lambda}| \frac{\partial\Psi j}{\partial\lambda}\} + \{ \Psi j \mid \frac{\partial^2 H}{\partial\lambda^2}|\Psi i \} = \frac{\partial^2 €_i}{\partial\lambda^2} \qquad (6)$$

Using the expansion (6); assuming for simplicity a discrete set of Eigen functions of H,

$$\frac{\partial\Psi j}{\partial\lambda} = \sum j\, \alpha ji\, \Psi j; \qquad (7)$$

and using the Hermiticity of $\frac{\partial H}{\partial\lambda}$, one can easily show that the derivatives of H with respect to the real parameter λ are all Hermitian

we obtain

$$\frac{1}{2}\frac{\partial^2 €i(\lambda)}{\partial\lambda^2} - \frac{1}{2}\{ \Psi j \mid \frac{\partial^2 H}{\partial\lambda^2}| \Psi i \} = \sum_j' \frac{h_{ij}h_{ji}}{(€_i €_j)}, \qquad (8)$$

Where $\sum_j'$ indicates summation over j excluding the j = I term and h = $\frac{\partial H}{\partial\lambda}$, so that

$$h_{ij} = \{ \Psi_i \mid \frac{\partial H}{\partial\lambda}|\Psi_i \} \qquad (9)$$

Upon differentiation of eqn (9) with respect to λ

We obtain,

$$\frac{\partial h_{ij}}{\partial\lambda} - \{ \Psi_i \mid \frac{\partial^2 H}{\partial\lambda^2}|\Psi_j \} = \sum_k (h_{ij}\, \alpha_{kj} - \alpha_{ik}\, h_{kj}) \qquad (10)$$

Further differentiating eq. (8) with respect to λ and using eq. (10) we can obtain, after some simplifications,

$\frac{1}{3!}\frac{\partial^3 €_i}{\partial\lambda^3} - \frac{1}{3!}\{ \Psi_i | \frac{\partial^3 H}{\partial\lambda^3}|\Psi_j \} - \frac{1}{2}\sum_k (h_{ij}^2 \alpha_{kj} - \alpha_{ik}h_{ji}^2)$

$= \sum_j'\sum_k' \frac{h_{ik}h_{kj}h_{ji}}{(€_j - €_i)(€_k - €_i)}$

$\frac{\partial €_i}{\partial\lambda^3}\sum_i' \frac{h_{ij}h_{ji}}{(€_k - €_i)^2} = \sum_i'\sum_k' \alpha_{ij}h_{jk}\alpha_{ki},$

Where

$h^{(2)} = \frac{\partial^2 H}{\partial\lambda^2}, \; h = \frac{\partial H}{\partial\lambda} - \frac{\partial €_i}{\partial\lambda}$

In this way we may proceed to obtain a series of sum rules involving matrix elements of the λ derivatives of the Hamiltonian H and its energy eigen value $€_i$. Our purpose for deriving these sum rules is to obtain the RS perturbation series in the limit λ —› 0, which we take up in Sec. III. It may be noted that in these sum rules only the non-diagonal co efficients α_{jk} appear.

3.Figures and Tables

The sum rules derived in sec.2 can be used to obtain the results of the RS perturbation theory [4, 5] and also the general result of LBW Perturbation theory in the form of a vanishing Hill determinant.

Suppose the Hamiltonian H(λ) cab be put in the form of

$H(\lambda) = H_0 + \lambda H'$,

Where λ is a continuously variable real parameter and H_0 and H' are independent of. Expanding the eigenvalue $€_i(\lambda)$ of H (λ) in Taylor series about λ= 0 we obtain

$$€_i(\lambda) = E_i + \lambda \frac{\partial €_i}{\partial\lambda} | \lambda = + (\lambda^2/2!) \frac{\partial^2 €_i}{\partial\lambda^2} | \lambda = + \ldots\ldots \quad (13)$$

Where $E_i = €_i (\lambda = 0)$ is an eigenvalue of H_0

$H_0 \Psi_i^0 = E_i \Psi_i^0$,

With $\Psi_i^0 = \Psi_i (\lambda = 0)$. The perturbation results are obtained simply by evaluating the λ derivatives at λ = 0. For the Hamiltonian (12) we also have

$\frac{\partial H}{\partial\lambda} = H', \frac{\partial^n H}{\partial\lambda^n} = 0$, for n≥2.

Suppose the unperturbed energy levels E_i are nondegenerate.

Taking the limit

$\lambda = 0$,

$h_{ij} (\lambda = 0) = \{ \Psi_i^{(0)} | H' | \Psi_j^{(0)} \} \equiv H'_{ij}$,

We obtain, from eqn (5), the first order perturbation energy

$$\Delta E_i^{(1)} = \{\Psi_i^{(0)} | H' | \Psi_j^{(0)}\} = H'_{ii} \quad (14)$$

From eqn (8), the second order perturbation energy

$$\Delta E_i^{(2)} = (1/2!)\frac{\partial €_i}{\partial\lambda}. | \lambda = 0 = \sum_j' \frac{H'_{ij}H'_{ji}}{(E_i - E_j)^2} \quad (15)$$

and from Eqn (11) the third order perturbation energy

$$\Delta E_i^{(3)} = (1/3!)\frac{\partial^3 €_i}{\partial\lambda^3} . | \lambda = 0 =$$

$$\sum_j'\sum_k' \frac{H'_{ij}H'_{jk}H'_{ki}}{(E_j - E_i)(E_k - E_i)} - \Delta E_i^{(1)} \sum_j' \frac{H'_{ij}H'_{ji}}{(E_i - E_j)^2} \quad (16)$$

Higher order energy can be readily found by further differentiation of Eqn (11) through the repeated use of Eqns (2) and (10) and then taking the λ = 0 limit. In this way we may obtain the energy of the perturbation in various orders by successive differentiation, without the necessity of explicit determination of the perturbed wave function.

4.Conclusion

In the present work, we have studied the Feynman Hellman theorem, Virial theorem and their applications. We started by giving somewhat detailed version of Epstein's extension of FH theorem and re-derivation of non-degenerate Ryleigh - Schrodinger perturbation expansion. We then studied virial theorem to calculate matrix elements of the kinetic and potential energies of a linear harmonic oscillator.

5.Acknowledgements

Thanks are due to department of Electrical Engineering, Narula Institute of Technology, West Bengal 700109 for providing the necessary facilities to carry out the research work.

References

This heading is not assigned a number.

[1] R. P. Feynman Phys Rev 56, 340(1939).
[2] H. Hellman, Einfuhrung in die Quantenchemte (Deuticke, Leipzing, 1937).
[3] S. Balasubramanium Am. J. Physics 5.2, 1143, (1984).
[4] H. S. Volk Am. J. Phys 54, 921 (1986).
[5] S. T. Epstein, Am. J. phys. Am - J - Phys 30, 266 (1962).
[6] B. H. Bransden and C. J. Joachin physics of atoms and molecules, PEARSON, Chapter 3, 2006