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Microarticle

# The Hellmann–Feynman theorem, the comparison theorem, and the envelope theory

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ABSTRACT

The envelope theory is a convenient method to compute approximate solutions for bound state equations in quantum mechanics. It is shown that these approximate solutions obey a kind of Hellmann–Feynman theorem, and that the comparison theorem can be applied to these approximate solutions for two ordered Hamiltonians.



The envelope theory (ET) [1–3], also known as the auxiliary field method [4–7], is a convenient method to compute approximate eigenvalues and eigenstates in quantum mechanics. The basic idea is to replace the Hamiltonian $H$ under study by an auxiliary Hamiltonian $\widetilde{H}$ which is solvable, the eigenvalues of $\widetilde{H}$ being optimized to be as close as possible to those of $H$. This method has several interesting characteristics: (i) Following the structure of the Hamiltonian $H$, the approximate eigenvalues can be upper or lower bounds, or not to have a variational character; (ii) The method is easy to implement since the solution can be obtained simply through a transcendental equation; (iii) The accuracy is reasonable and can be improved by fitting one parameter introduced in the global quantum numbers. In this paper, it is shown that the approximate solutions obey a kind of Hellmann–Feynman theorem [8–10], and that the comparison theorem [11,12] can be applied to approximate solutions for two ordered Hamiltonians.

Let us assume that the Hamiltonian $H$ for $N$ identical particles can be written as ($\hbar = c = 1$)

$$H = \sum_{i=1}^{N} T(|\boldsymbol{p}_i|) + \sum_{i=1}^{N} U(|\boldsymbol{r}_i - \boldsymbol{R}|) + \sum_{i<j=2}^{N} V(|\boldsymbol{r}_i - \boldsymbol{r}_j|). \tag{1}$$

$T$ is a kinetic energy, $U$ a one-body interaction, $V$ a two-body potential and $\boldsymbol{R} = \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{r}_i$ is the center of mass position. In the framework of ET, an approximate eigenvalue $E$ is given by the following equation for a completely (anti)symmetrised state and the center of mass motion removed $\left(\sum_{i=1}^{N} \boldsymbol{p}_i = \boldsymbol{0}\right)$ [5]

$$E = NT(p_0) + NU\left(\frac{r_0}{N}\right) + C_N V\left(\frac{r_0}{\sqrt{C_N}}\right), \tag{2}$$

where $C_N = N(N-1)/2$ is the number of particle pairs, $p_0$ is the mean momentum per particle and $r_0/N$ the radius of the system. $p_0$ and $r_0$ are linked by the following relation

$$r_0 p_0 = Q, \tag{3}$$

where

$$Q = \sum_{i=1}^{N-1} (\phi n_i + l_i) + (N-1)\frac{D+\phi-2}{2} \tag{4}$$

is a global quantum number in $D$ dimensions. In the original method, $\phi = 2$, which corresponds to the global quantum number of $N-1$ identical harmonic oscillators. It has been shown that allowing variations of $\phi$ can improve the accuracy of the approximate eigenvalues [6,7]. In this case, the variational character of the solution cannot be guaranteed. The parameter $r_0$ is the solution of the equation

$$\left.\frac{\partial E}{\partial r_0}\right|_{p_0 = Q/r_0} = 0. \tag{5}$$

Let us note that (5) is the translation into variables $r_0$ and $p_0$ of the generalized virial theorem [13].

The Hellmann–Feynman theorem states that if the Hamiltonian of a system $H(\mu)$ depends on a parameter $\mu$, and that the eigenvalue equation for a bound state is

$$H(\mu)|\mu\rangle = E(\mu)|\mu\rangle, \tag{6}$$

where $E(\mu)$ is the energy and $|\mu\rangle$ the normalized associated eigenstate, then

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$$\frac{dE(\mu)}{d\mu} = \left\langle \mu \left| \frac{\partial H(\mu)}{\partial \mu} \right| \mu \right\rangle. \tag{7}$$

Solving system (2)–(5) for such a Hamiltonian $H(\mu)$, one finds $E = E(\mu, r_0)$ with $r_0 = r_0(\mu)$. One can then write $E = E(\mu, r_0(\mu))$. The variation of the eigenvalue with $\mu$ is given by

$$\frac{dE}{d\mu} = \frac{\partial E}{\partial \mu} + \frac{\partial E}{\partial r_0}\frac{\partial r_0}{\partial \mu}. \tag{8}$$

With relation (5), one finally gets

$$\frac{dE}{d\mu} = \left.\frac{\partial E}{\partial \mu}\right|_{r_0 = r_0(\mu)}. \tag{9}$$

This relation can be useful to easily compute $dE/d\mu$ if $r_0$ is only known numerically. It can be considered as the translation into variables $r_0$ and $p_0$ of the Hellmann–Feynman theorem. This theorem shows that the variation of the eigenvalue can be obtained by computing the partial derivative of the Hamiltonian, and by computing its mean value for the eigenstate considered. For ET, the variation of the eigenvalue can be obtained by computing the partial derivative of the form (2) giving the approximate eigenvalue, and by computing its value for the parameter $r_0$ of the approximate state considered.

The comparison theorem states that if two Hamiltonians $H^{(1)}$ and $H^{(2)}$ are ordered, $\langle\phi|H^{(1)}|\phi\rangle \leqslant \langle\phi|H^{(2)}|\phi\rangle$ for any state $|\phi\rangle$, then each corresponding pair of eigenvalues is ordered $E^{(1)} \leqslant E^{(2)}$, for the same set of quantum numbers [11,12].

Let us follow the procedure established in [12] by assuming that the Hamiltonian

$$H(\mu) = (1-\mu)H^{(1)} + \mu H^{(2)} \tag{10}$$

possesses a number (finite or infinite) of well defined eigenvalues $E(\mu)$ for $0 \leqslant \mu \leqslant 1$. An approximate solution for a given state computed by ET is

$$E(\mu, r_0(\mu)) = (1-\mu)E^{(1)}(r_0(\mu)) + \mu E^{(2)}(r_0(\mu)), \tag{11}$$

where $E^{(i)}(r_0(\mu))$ is the form (2) for a Hamiltonian $H^{(i)}$. From Eq. (9), it appears that

$$\frac{dE}{d\mu} = E^{(2)}(r_0(\mu)) - E^{(1)}(r_0(\mu)). \tag{12}$$

In order to be sure that the two Hamiltonians are ordered, it is necessary that the following three conditions $\{T^{(1)}(x) \leqslant T^{(2)}(x), U^{(1)}(x) \leqslant U^{(2)}(x), V^{(1)}(x) \leqslant V^{(2)}(x)\}$ are all fulfilled [12]. In this case, $dE/d\mu \geqslant 0$. Consequently,

$$E^{(1)}(r_0(\mu = 0)) \leqslant E^{(2)}(r_0(\mu = 1)), \tag{13}$$

where $E^{(1)}(r_0(\mu = 0))$ and $E^{(2)}(r_0(\mu = 1))$ are respectively the approximate eigenvalues, with the same quantum numbers, for Hamiltonians $H^{(1)}$ and $H^{(2)}$. The approximate eigenvalues computed by ET are then also ordered. This does not mean that the quality of the approximation is the same for the two Hamiltonians $H^{(i)}$, but at least the hierarchy of the approximate eigenvalues corresponds to the hierarchy of the genuine eigenvalues.

## References


[1] Hall RL. Phys Rev D 1980;22:2062.
[2] Hall RL. J Math Phys 1983;24:324.
[3] Hall RL, Lucha W, Schöberl FF. J Math Phys 2004;45:3086.
[4] Silvestre-Brac B, Semay C, Buisseret F, Brau F. J Math Phys 2010;51:032104.
[5] Semay C, Roland C. Results Phys 2013;3:231.
[6] Semay C. Few-Body Syst 2015;56:149.
[7] Semay C. Eur Phys J Plus 2015;130:156.
[8] Hellmann H. Acta Physicochimica URSS 1935;1:913.
[9] Feynman RP. Phys Rev 1939;56:340.
[10] Lichtenberg DB. Phys Rev D 1989;40:4196.
[11] Reed M, Simon B. Methods of modern mathematical physics. IV. analysis of operators. New York: Academic Press; 1978.
[12] Semay C. Phys Rev A 2011;83:024101.
[13] Lucha W. Mod Phys Lett A 1990;5:2473.