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Generalisation of the Hellmann–Feynman theorem to Gamow states

P Ziesche†§, K Kunze‡ and B Milek‡

† International Centre for Theoretical Physics, Miramare, Trieste, Italy
‡ Technische Universität Dresden, Sektion Physik, Mommsenstrasse 13, Dresden-8027, German Democratic Republic

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Abstract. The Hellmann-Feynman theorem valid for the parameter dependence of bound states is generalised to the case of Gamow states using an appropriate definition of scalar products and expectation values with such states. The one-dimensional square well potential is considered as an illustrative example.

1. Introduction

There has been recent interest in the Pauli-Hellmann-Feynman theorem (PHFT) and its applications within solid state theory and quantum chemistry to (i) inhomogeneous jellia including spheres, voids, adsorption and forces on and between jellia [1-6], (ii) forces and pressure in solids [7], (iii) phonon energies in semiconductors [8], (iv) relaxation of metal surfaces [9], (v) point defects in metals [10] and semiconductors [11], (vi) the gauge treatment of the quantum Hall effect [12], and (vii) clusters [13]. It is mentioned in connection with the stress theorem [14] and it has a relationship with the force theorem [15]. The PHFT (first found by Pauli, see, e.g., [3] or [14]) states the following: if a system described by a Hamiltonian $H(\lambda)$, where λ is a certain parameter, has bound states φ_n, E_n, then it is

$$\frac{\mathrm{d}E_n}{\mathrm{d}\lambda}=\frac{\langle\varphi_n|\mathrm{d}H/\mathrm{d}\lambda|\varphi_n\rangle}{\langle\varphi_n|\varphi_n\rangle}. \tag{1.1}$$

If λ means, for example, the position of a nucleus (within the Born-Oppenheimer approximation of clusters or solids), then on the RHS a PHF force appears, driving a relaxation. The parameter may also be a coupling constant, e.g. the well known 'charging formula' within the many-body theory of the electron gas ground state ϕ

$$E(\lambda)-E(0)=\int_0^\lambda \frac{\mathrm{d}\lambda}{\lambda}\langle\phi|V|\phi\rangle/\langle\phi|\phi\rangle \tag{1.2}$$

where $H=H^0+V$, $V\sim\lambda=e^2/4\pi\varepsilon_0$, rests upon the PHFT (see, e.g., [16]).

The question arises if an appropriately generalised version of the PHFT can be derived also for scattering states. For the continuum of scattering states there does

§ Permanent address: Technische Universität Dresden, Sektion Physik, Mommsenstrasse 13, Dresden-8027, German Democratic Republic.

not exist any parameter dependence $E(\lambda)$, but the complex energies $E_n^{\pm}$ of the discrete Gamow states (see § 2) of course depend on λ and it is natural to ask for $\mathrm{d}E_n^{\pm}/\mathrm{d}\lambda$ (see § 3). For simplicity we restrict ourselves to single-particle problems. The result (3.3) will be illustrated by a simple example (§ 4).

2. Gamow states

Quasistationary states were introduced in nuclear physics by Gamow long ago in order to describe the α-decay phenomenon [17]. After that a lot of attempts were made to introduce such resonant states in formal nuclear reaction theories (see, e.g., [18]) as well as in practical calculations [19].

Gamow states are defined as solutions of the stationary Schrödinger equation satisfying the asymptotic boundary conditions of purely outgoing (+) or purely incoming (−) waves. These conditions makes the problem non-self-adjoint. Hence the energy eigenvalues of the adjoint states according to

$$H|\varphi_n^+\rangle = E_n^+|\varphi_n^+\rangle \tag{2.1a}$$

$$H^{+}|\varphi_n^-\rangle = E_n^-|\varphi_n^-\rangle \tag{2.1b}$$

are complex ($E_n^{\pm} = E_n \mp \mathrm{i}\Gamma_n$ with $\Gamma_n > 0$), and the Gamow states are not normalisable and orthogonal in the usual sense because of the divergence of the amplitudes for large distances.

In an equivalent way to (2.1), the problem may be formulated by a homogeneous Lippmann–Schwinger equation

$$|\varphi^{\pm}(E)\rangle = G_0^{\pm}(E)V|\varphi^{\pm}(E)\rangle \qquad G_0^{\pm}(E) = (E - \boldsymbol{p}^2/2M \pm \mathrm{i}\delta)^{-1} \tag{2.2}$$

where $\boldsymbol{p}$ is the momentum operator, $G_0^{\pm}(E)$ is the free particle Green operator and $\delta \gtrless 0$ expresses the desired asymptotic behaviour. The condition

$$\det\|1 - G_0^{\pm}(E)V\| = 0 \tag{2.3}$$

needed in order to obtain non-trivial solutions of (2.2), cannot be fulfilled by any real energy E. However, after calculating the matrix elements of $G_0^{\pm}(E)$, taking the δ limit and performing an analytic continuation to the complex E plane according to $E \to E \mp \mathrm{i}\Gamma$, (2.3) becomes complex and yields E_n and Γ_n, the position and decay width of the Gamow state, respectively. Finally from (2.2) one obtains the corresponding wavefunctions $\varphi_n^{\pm} = \varphi^{\pm}(E_n^{\pm})$. The whole procedure can be formulated in a compact form as

$$G_0^{\pm}(E_n^{\pm}) = \left[\lim_{\delta \gtrless 0}\left(E - \frac{\boldsymbol{p}^2}{2M} \pm \mathrm{i}\delta\right)^{-1}\right]_{E \to E_n^{\pm}} \tag{2.4}$$

stressing the fact that an interchange of the δ limit and the analytic continuation would give the wrong results (for example, incoming waves with exponentially decaying amplitude instead of the desired outgoing waves).

Recently [20] a generalised scalar product of an outgoing and an incoming Gamow state was defined in an analogous way:

(i) calculating the integrals occurring with an energy $E + \mathrm{i}\delta$ for the outgoing and $E - \mathrm{i}\delta$ for the incoming state,

(ii) taking the δ limit,

(iii) performing the analytic continuation to the complex E plane with $E \to E_n^{\pm} = E_n \mp i\Gamma_n$.

In this way it has been shown that the Gamow states form a biorthogonal set

$$\langle \varphi_n^- | \varphi_{n'}^+ \rangle \sim \delta_{nn'} \tag{2.5}$$

and a proper norm has also been introduced. Generalised 'expectation values' $\langle \varphi_n^- | A | \varphi_n^+ \rangle / \langle \varphi_n^- | \varphi_n^+ \rangle$ can be defined similarly.

We would like to mention that Gamow states, bound states and suitably chosen scattering states within the proposed treatment fulfil a completeness relation [20].

3. The PHFT for Gamow states

If $H = H(\lambda)$ then the Gamow states $\varphi_n^{\pm}$, $E_n^{\pm}$ depend on the parameter λ, too. From

$$E_n^+ = \frac{\langle \varphi_n^- | H | \varphi_n^+ \rangle}{\langle \varphi_n^- | \varphi_n^+ \rangle} \tag{3.1}$$

one obtains easily

$$\frac{dE_n^+}{d\lambda} \langle \varphi_n^- | \varphi_n^+ \rangle + E_n^+ \frac{d}{d\lambda} \langle \varphi_n^- | \varphi_n^+ \rangle = \left\langle \frac{d\varphi_n^-}{d\lambda} \middle| H \middle| \varphi_n^+ \right\rangle + \left\langle \varphi_n^- \middle| H \middle| \frac{d\varphi_n^+}{d\lambda} \right\rangle + \left\langle \varphi_n^- \middle| \frac{dH}{d\lambda} \middle| \varphi_n^+ \right\rangle. \tag{3.2}$$

Using (2.1) and the identity $E_n^+ = (E_n^-)^*$, the final result is

$$\frac{dE_n^+}{d\lambda} = \frac{\langle \varphi_n^- | dH/d\lambda | \varphi_n^+ \rangle}{\langle \varphi_n^- | \varphi_n^+ \rangle} \tag{3.3a}$$

$$\frac{dE_n^-}{d\lambda} = \frac{\langle \varphi_n^+ | dH^+/d\lambda | \varphi_n^- \rangle}{\langle \varphi_n^+ | \varphi_n^- \rangle}. \tag{3.3b}$$

This is the extension of the PHFT to Gamow states.

Comparing (1.1) and (3.3) the theorems are quite similar, except that for Gamow states on the RHS a generalised expectation value is introduced. As mentioned in § 1 the PHFT for bound states is a useful tool (at least as a rigorous sum rule). The same statement may be true for Gamow states because they influence the scattering properties for real energies as poles of the S matrix.

If $E_n^{\pm}(\lambda)$ changes in such a way that, for a certain critical value λ_c, the Gamow state n transforms itself into a bound state as was seen, e.g., in [19, 20], then (3.3) should also turn into (1.1).

A special case of Gamow states appears if single atoms, clusters or spherical jellia are considered to be in a homogeneous weak external electric field. Bound states principally do not exist further on. They turn into Gamow states, the energies of which have very small imaginary parts, describing the successive tunnelling away of all initially bound electrons with a very small probability. Now (3.3) should allow the PHFT to be applied to such cases (in [5] a jellium sphere in an external electric field was considered).

Excited states of atoms because of their coupling to the radiation field should be understood principally as Gamow states, to which (3.3) should also be applicable.

4. An illustrative example

In this section the validity of the PHFT for Gamow states will be demonstrated for the simple example of a quantum well $V(x) = -(\hbar^2/2m)v\theta(a-|x|)$.

According to the definition of §2 one obtains the Gamow states in space representation

$$\varphi_n^\pm(x) = [\lim_{\delta \gtrless 0} \varphi^\mp(x;\, k \pm \mathrm{i}\delta)]_{k\to k_n^\mp} \tag{4.1}$$

with

$$\varphi^\pm(x;\, k) = \begin{cases} \dfrac{1}{\sqrt{a}} \sin Kx & |x| \leqslant a \\ \dfrac{1}{\sqrt{a}} \dfrac{x}{|x|} \sin Ka \exp(\pm \mathrm{i}k(|x|-a)) & |x| > a \end{cases} \tag{4.2}$$

where k real, $K = K(k)$ with $K^2 = k^2 + v$, and only antisymmetric states are considered. The complex wavenumbers $k_n^\mp = R_n \mp I_n$ $(R_n, I_n > 0)$ are discrete solutions of the transcendental equation

$$K \cos Ka \mp \mathrm{i}k \sin Ka = 0 \tag{4.3}$$

(see [21]). The wavefunctions (4.1) solve the stationary Schrödinger equation and satisfy for these wavenumbers k_n^+ and k_n^- the asymptotic boundary condition of purely outgoing or incoming waves, respectively.

However, if these complex numbers $k_n^\pm$ are immediately inserted in the wavefunctions (4.2) before taking the δ limit the well known exponentially increasing amplitude would be created, which leads to divergent integrals when forming a norm or scalar products. That is why the Gamow states are represented according to (4.1) as operators, which allow us to define a proper scalar product of two Gamow states as follows:

$$\langle \varphi_n^- | \varphi_{n'}^+ \rangle = \left(\lim_{\delta \gtrless 0} \int_{-\infty}^{+\infty} \mathrm{d}x (\varphi^-(x;\, k-\mathrm{i}\delta))^* \varphi^+(x;\, k'+\mathrm{i}\delta) \right)_{\substack{k\to(k_n^-)^* \\ k'\to k_{n'}^+}}. \tag{4.4}$$

Thereby expressions occurring of the following type (note that $\varphi^{-*} = \varphi^+$) give

$$\lim_{\delta \gtrless 0} \frac{1}{a} \int_a^\infty \mathrm{d}x \{\exp[-\mathrm{i}(k-\mathrm{i}\delta)(x-a)]\}^* \exp[\mathrm{i}(k'+\mathrm{i}\delta)(x-a)] = -\frac{1}{\mathrm{i}(k+k')a}. \tag{4.5}$$

The complete calculation of the scalar product (4.4) leads to the biorthogonality relation

$$\langle \varphi_n^- | \varphi_{n'}^+ \rangle = \left(1 - \frac{1}{\mathrm{i}k_n^+ a}\right) \delta_{nn'}. \tag{4.6}$$

In the same way one obtains (using (4.3))

$$\frac{\langle \varphi_n^- | \mathrm{d}H/\mathrm{d}v | \varphi_n^+ \rangle}{\langle \varphi_n^- | \varphi_n^+ \rangle} = -\frac{\hbar^2}{2m} \frac{\cos^2 K_n^+ a - \mathrm{i}k_n^+ a}{1 - \mathrm{i}k_n^+ a}. \tag{4.7}$$

On the other hand, (4.3) yields

$$(K_n^+)^2 \cot^2 K_n^+ a = -(k_n^+)^2 \tag{4.8}$$

and by an implicit differentiation of (4.8)

$$\left(\frac{2m}{\hbar^2} \frac{\mathrm{d}E_n^+}{\mathrm{d}v} + 1\right)\left(\cot^2 K_n^+ a - \frac{K_n^+ a \cot K_n^+ a}{\sin^2 K_n^+ a}\right) = -\frac{2m}{\hbar^2} \frac{\mathrm{d}E_n^+}{\mathrm{d}v} \tag{4.9}$$

with $E_n^+ = (\hbar^2/2m)(k_n^+)^2$. Finally the same result as in (4.7) follows for dE_n^+/dv, as it should because of the PHFT (3.3).

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