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GENERALIZATION OF THE HELLMANN-FEYNMAN THEOREM TO GAMOW STATES*

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ABSTRACT

The Hellmann-Feynman theorem valid for the parameter dependence of bound states is generalized 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 illustrating example.

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1. INTRODUCTION

There is a 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/, (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

$$\frac{dE_n}{d\lambda} = \frac{\langle\varphi_n|dH/d\lambda|\varphi_n\rangle}{\langle\varphi_n|\varphi_n\rangle} . \tag{1.1}$$

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

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

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 generalized version of the PHFT can be derived also for scattering states. For the continuum of scattering states there does not exist any parameter dependence $E(\lambda)$, but the complex energies $E_n^{\pm}$ of the discrete Gamow states (see Sec.2) of course depend on λ and it is naturally to ask for $dE_n^{\pm}/d\lambda$ (see Sec.3). For simplicity we restrict ourselves to single particle problems. The result (3.3) will be illustrated by a simple example (Sec.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 performed 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 make the problem non-self- adjoint. Hence the energy eigenvalues of the adjoint states according to

$$H|\varphi_n^+\rangle = E_n^+|\varphi_n^+\rangle \quad , \quad H^\dagger|\varphi_n^-\rangle = E_n^-|\varphi_n^-\rangle \qquad (2.1a,b)$$

are complex ($E_n = E_n \mp i\Gamma_n$ 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.

Equivalently to Eqs. (2.1) the problem may be formulated by a homogeneous Lippmann-Schwinger equation

$$|\varphi^\pm(E)\rangle = G_0^\pm(E)V|\varphi^\pm(E)\rangle \ , \quad G_0^\pm(E) = \left(E - \frac{p^2}{2m} \pm i\delta\right)^{-1} , \ \delta \gtrsim 0 , \qquad (2.2)$$

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

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

in order to get non-trivial solutions of (2.2) cannot be fulfilled by any real energy E. But after calculating the matrix elements of $G_0^\pm(E)$, taking the δ-limit, performing an analytic continuation to the complex E plane according to $E \to E \mp i\Gamma$, Eq. (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 gets the corresponding wave functions $\varphi_n^\pm = \varphi^\pm(E_n^\pm)$.

The whole procedure can be formulated in an compact form as

$$G_0^\pm(E_n^\pm) = \left[\lim_{\delta \gtrsim 0}\left(E - \frac{p^2}{2m} \pm i\delta\right)\right]_{E \to E_n^\pm} , \qquad (2.4)$$

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

Recently /20/ a generalised scalar product of an outgoing and an incoming Gamow state were defined in an analogous way,

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

(ii) taking the δ-limit,

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

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

$$\langle\varphi_n^-|\varphi_{n'}^+\rangle \sim \delta_{nn'} , \qquad (2.5)$$

and a proper norm has also been introduced. Generalized "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 suitable choosen 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

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

one easily obtains

$$\frac{dE_n^+}{d\lambda}\langle\varphi_n^-|\varphi_n^+\rangle + E_n^+\frac{d}{d\lambda}\langle\varphi_n^-|\varphi_n^+\rangle$$

$$= \langle\frac{d\varphi_n^-}{d\lambda}|H|\varphi_n^+\rangle + \langle\varphi_n^-|H\frac{d\varphi_n^+}{d\lambda}\rangle + \langle\varphi_n^-|\frac{dH}{d\lambda}|\varphi_n^+\rangle . \qquad (3.2)$$

Using Eqs. (2.1) and the identity $E_n^+ = (E_m^-)^*$ finally it results

$$\frac{dE_n^+}{d\lambda} = \frac{\langle\varphi_n^-|dH/d\lambda|\varphi_n^+\rangle}{\langle\varphi_n^-|\varphi_n^+\rangle} \quad , \quad \frac{dE_n^-}{d\lambda} = \frac{\langle\varphi_n^-|dH/d\lambda|\varphi_n^+\rangle}{\langle\varphi_n^-|\varphi_n^+\rangle} . \qquad (3.3a,b)$$

This is the extension of the PHFT to Gamow states.

Comparing (1.1) and (3.3) the theorems are quite similar, only for Gamow states on the r.h.s. a generalized expectation value is introduced. As mentioned in Sec. 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 as poles of the S-Matrix the scattering properties for real energies.

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 it was seen e.g. in /19,20/, then also (3.3) should turn into (1.1).

A special case of Gamow states appears if single atoms, clusters or spherical jellia are considered to be in an 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 tunneling away of all initially bound electrons with a very small probability. Now (3.3) should allow to apply the PHFT 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 Eq. (3.3) should be applicable, too.

4. AN ILLUSTRATING 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 Sec. 2 one gets the Gamow states in space representation

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

with

$$\varphi^{\pm}(x;k) = \begin{cases} \frac{1}{\sqrt{a}} \sin Kx & |x|\le a \\ \frac{1}{\sqrt{a}}\frac{x}{|x|} \sin Ka \quad \exp\left(\pm ik(|x|-a)\right) & |x|>a \end{cases} \tag{4.2}$$

where k real, $K = K(k)$ with $K^2 = k^2+v$, and antisymmetric states are considered only. The complex wave numbers $k_n^{\pm} = R_n \mp iI_n$ $(R_n, I_n > 0)$ are discrete solutions of the transcendent equation

$$K \cos Ka \mp ik \sin Ka = 0 \tag{4.3}$$

(see /21/). The wave functions (4.1) solve the stationary Schrödinger equation and satisfy for these wave numbers k_n^+ and k_n^- the asymptotic boundary condition of purely outgoing or incoming waves, respectively.

But if these complex numbers $k_n^{\pm}$ are immediately inserted in the wave functions (4.2) before taking the δ-limit the well known exponential 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 Eq. (4.1) as operators, which allow to define a proper scalar product of two Gamow states as follows:

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

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

$$\lim_{\delta\to 0} \frac{1}{a}\int_a^\infty dx \left(e^{-i(k-i\delta)(x-a)}\right)^* e^{+i(k'+i\delta)(x-a)} = -\frac{1}{i(k+k')a} \quad . \tag{4.5}$$

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

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

In the same way one gets (using Eq.(4.3))

$$\frac{\langle \varphi_n^- | dH/dv | \varphi_n^+ \rangle}{\langle \varphi_n^- | \varphi_n^+ \rangle} = -\frac{\hbar^2}{2m} \frac{\cos^2 K_n^+ a - ik_n^+ a}{1 - ik_n^+ a} \quad . \tag{4.7}$$

On the other hand Eq.(4.3) yields

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

and by an implicite differentation of Eq. (4.8)

$$\left(\frac{2m}{\hbar^2}\frac{dE_n^+}{dv} + 1\right)\left(\cot^2 K_n^+ a - \frac{K_n^+ a \cot K_n^+ a}{\sin^2 K_n^+ a}\right) = -\frac{2m}{\hbar^2}\frac{dE_n^+}{dv} \tag{4.9}$$

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

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