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Application of a generalized Feynman-Hellmann theorem to bound-state energy levels

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We derive a generalization of the Feynman-Hellmann theorem and use it to describe how the energy of a bound state changes with the change in mass of one of the constituent particles.

Quigg and Rosner[1] have applied a theorem of Feynman[2] and Hellmann[3] (FH) to the energy levels of bound states in a potential. Specifically, Quigg and Rosner used the FH theorem to show that the larger the reduced mass of two nonrelativistic particles bound in a potential, the lower a specified bound state lies in that potential. In this paper, we use a generalized FH theorem to show that the energy levels (excluding the rest energy) of bound states decrease with increasing mass of any constituent particle for certain relativistic wave equations. We also show that this result is not necessarily true for all wave equations incorporating relativistic kinematics.

The motivation of Quigg and Rosner was to obtain results for quarkonium which depend on quark masses but not on the functional form of the potential between the quark and antiquark. Subsequently, other authors[4] applied the theorem to obtain inequalities among quark and hadron masses. Our motivation is similar to that of previous authors, but we do not wish to restrict ourselves to the nonrelativistic Schrödinger equation or to bound states of only two particles.

The Feynman-Hellmann theorem states that if the Hamiltonian of a system is $H(\lambda)$, where λ is a parameter, and the wave equation for a bound state is

$$H(\lambda)\psi(\lambda)=E(\lambda)\psi(\lambda)\ , \qquad (1)$$

where E is the energy and ψ is a normalized wave function, then

$$\frac{\partial E}{\partial \lambda}=\left\langle \psi \left| \frac{\partial H}{\partial \lambda} \right| \psi \right\rangle . \qquad (2)$$

There are certain relativistic wave equations, such as the Klein-Gordon equation, which are not of the form of Eq. (1), so that the FH theorem does not directly apply. However, we shall generalize the FH theorem to a form which can apply to the Klein-Gordon equation and a class of other relativistic wave equations.

We consider a wave equation of the form

$$F(E,\lambda)\psi=0\ , \qquad (3)$$

where ψ is the wave function of a bound state with energy E, which depends on the parameter λ. Then we can write

$$\frac{\partial}{\partial \lambda}\langle \psi|F|\psi\rangle=\left\langle \frac{\partial \psi}{\partial \lambda} \left| F \right| \psi \right\rangle+\left\langle \psi \left| \frac{\partial F}{\partial E}\frac{\partial E}{\partial \lambda}+\frac{\partial F}{\partial \lambda} \right| \psi \right\rangle + \left\langle \psi \left| F \right| \frac{\partial \psi}{\partial \lambda} \right\rangle=0\ . \qquad (4)$$

If F has the property that

$$\left\langle \psi \left| F \right| \frac{\partial \psi}{\partial \lambda} \right\rangle=\left\langle F\psi \left| \frac{\partial \psi}{\partial \lambda} \right.\right\rangle , \qquad (5)$$

then, in view of Eq. (3), Eq. (4) becomes

$$\left\langle \psi \left| \frac{\partial F}{\partial E}\frac{\partial E}{\partial \lambda}+\frac{\partial F}{\partial \lambda} \right| \psi \right\rangle=0$$

or

$$\frac{\partial E}{\partial \lambda}=-\left\langle \psi \left| \frac{\partial F}{\partial \lambda} \right| \psi \right\rangle \Big/ \left\langle \psi \left| \frac{\partial F}{\partial E} \right| \psi \right\rangle . \qquad (6)$$

If $F=H-E$, then Eq. (6) reduces to the form given in Eq. (2), provided $\langle \psi|\psi\rangle=1$, as we shall require. Equation (6) is our generalization of the FH theorem. We have not seen it elsewhere in the literature, although it is related to ideas presented in papers by Klein and Rafelski[5] and by Epstein.[6]

In applying Eqs. (2) and (6) to determine how the energy of a bound state varies with the mass of one of its constituent particles, we shall take E to be the total energy including the rest energy and require that $E>0$. We define ϵ to be $\epsilon=E-\sum_i m_i$, where m_i are the masses of the constituents. The statement that as the mass m_i of any constituent increases, the bound state lies lower in the potential means that

$$\frac{\partial \epsilon}{\partial m_i}<0\ . \qquad (7)$$

It follows from the FH theorem [Eq. (2)] that the inequality (7) holds for the n-body Schrödinger equation, provided that the potential does not depend on the constituent masses. We do not present the proof, as it is a straightforward generalization of that given in Quigg and Rosner.[1] We assume in what follows that all potentials are independent of masses.

Let us now apply Eq. (2) to a particle of mass m satisfying the Dirac equation with a potential S which transforms like a Lorentz scalar and a potential V which transforms like the zeroth component of a Lorentz four-vector. The equation is of the form ($\hbar=c=1$)

$$[\boldsymbol{\alpha}\cdot\mathbf{p}+\beta(m+S)]\psi=(E-V)\psi\ , \qquad (8)$$

where α and β are Dirac matrices and $\mathbf{p}=-i\nabla$. Using Eq. (2), we obtain

$$\frac{\partial E}{\partial m}=\langle \psi|\beta|\psi\rangle \ . \tag{9}$$

But for a normalized bound state, we have $\langle \psi|\beta|\psi\rangle < 1$, so that we obtain

$$\frac{\partial E}{\partial m}<1 \ . \tag{10}$$

The generalization to a bound state of n Dirac particles bound in potentials V and S is straightforward if the wave equation is of the form

$$\sum_i [\boldsymbol{\alpha}_i\cdot\mathbf{p}_i+\beta_i(m_i+S_i)]\psi=(E-V)\psi \ .$$

Then Eq. (7) holds, just as with the nonrelativistic Schrödinger equation.

We next consider the n-body spinless Salpeter equation, given by

$$\sum_i [(\mathbf{p}_i^2+m_i^2)^{1/2}+V]\psi=E\psi \ . \tag{11}$$

Again using Eq. (2), we obtain

$$\frac{\partial E}{\partial m_i}=m_i\langle \psi|(\mathbf{p}_i^2+m_i^2)^{-1/2}|\psi\rangle <1 \ , \tag{12}$$

because $\mathbf{p}_i^2$ is a positive-definite operator (in momentum space $\mathbf{p}_i^2$ is a positive multiplicative operator). It follows that the inequality (7) again holds.

We now turn to the Klein-Gordon equation, which we write in the form

$$[\mathbf{p}^2+(m+S)^2-(E-V)^2]\psi=0 \ . \tag{13}$$

Using Eq. (6), we obtain

$$\frac{\partial E}{\partial m}=\frac{m+\langle \psi|S|\psi\rangle}{E-\langle \psi|V|\psi\rangle} \ . \tag{14}$$

It is not obvious in this case whether $\partial E/\partial m$ is greater or less than 1. However, we can show in the case $V=0$, that the inequalities (10) and (7) hold.

The proof is as follows. Because $\mathbf{p}^2$ is a positive-definite operator, we see from Eq. (13) that if $V=0$, we have

$$E^2>\langle \psi|(m+S)^2|\psi\rangle \ . \tag{15}$$

Now a theorem tells us that for a Hermitian operator U, we have

$$\langle \psi|U^2|\psi\rangle \geq (\langle \psi|U|\psi\rangle)^2 \ .$$

Therefore, we obtain

$$(m+\langle \psi|S|\psi\rangle)^2\leq \langle \psi|(m+S)^2|\psi\rangle \ . \tag{16}$$

Setting $V=0$ in Eq. (14) and using (15) and (16), we obtain the inequality (10). Then the inequality (7) follows immediately from the definition of ϵ. An analogous proof follows for the Klein-Gordon equation for two particles of equal mass.

Let us next consider a simple way to introduce relativistic kinematics into the Schrödinger equation. We restrict ourselves here to the one-body case, which is sufficient to demonstrate that, for the prescription given below, the quantity $\partial\epsilon/\partial m$ is not necessarily negative. We write the Schrödinger equation in the form

$$(\mathbf{p}^2+2mV)\psi=k^2\psi \ , \tag{17}$$

where k^2 is the momentum-squared eigenvalue, and let E be given by

$$E=(m^2+k^2)^{1/2} \ . \tag{18}$$

The eigenvalue k^2 may be either positive or negative, but must satisfy the inequality $k^2>-m^2$ so that $E>0$. Note that if $|k^2|$ is much smaller than m^2, Eq. (18) reduces to the usual nonrelativistic expression for the energy: $\epsilon=k^2/(2m)$. Using Eq. (6), we obtain, from Eqs. (17) and (18),

$$\frac{\partial E}{\partial m}=\frac{m+\langle \psi|V|\psi\rangle}{E} \ . \tag{19}$$

We can use Eq. (19) to show explicitly that potentials exist for which the inequalities (7) and (10) are violated. For example, for a potential of the form $V=ar^2$, we can evaluate E and $\langle \psi|V|\psi\rangle$ analytically for a given energy level to show that (7) and (10) do not hold for sufficiently large am^3. Alternatively, we can make use of the scaling properties of the Schrödinger equation with a power-law potential.[1] These properties enable us to show directly that if E is given by Eq. (18) and if

$$V=ar^b, \quad ab>0, \quad b>-1 \ ,$$

then, for a given m and b, we can choose a so that the inequalities (7) and (10) do not hold for some energy levels. Of course, the inequalities hold if E is given by the usual nonrelativistic expression $E=m+k^2/(2m)$.

In conclusion, we have applied a generalized Feynman-Hellmann theorem to the problem of particles bound in a potential which is independent of the constituent masses. We have shown that for the nonrelativistic Schrödinger equation and for some, but not all, relativistic wave equations, a bound-state energy ϵ (excluding the rest energy) decreases as the mass of any constituent particle increases. If ϵ increases as a constituent mass increases, then of course the total energy E (including the rest energy) will also increase. However, if ϵ decreases as a constituent mass increases, we cannot say in general whether the total energy E increases or decreases. Whether $\partial E/\partial m_i$ is greater or less than zero depends on the form of the potential as well as on the wave equation.

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