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THE RELATIVISTIC VIRIAL THEOREM

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Abstract

The relativistic generalization of the quantum-mechanical virial theorem is derived and used to clarify the connection between the nonrelativistic and (semi-)relativistic treatment of bound states.

It has been a long-standing puzzle in hadron spectroscopy why the description of hadrons containing light quarks by two seemingly different approaches, viz. in terms of the nonrelativistic Schrödinger formalism on the one hand [1,2] and by a semirelativistic Hamiltonian incorporating relativistic kinematics on the other hand [3,4,5,6], produces comparably good results. In this note we derive a relation which may be regarded as the relativistic generalization of the virial theorem well known in nonrelativistic quantum mechanics. With this relativistic virial theorem at our disposal we are able to cast some light on the above-mentioned puzzle.

Consider the two-particle Hamiltonian with relativistic kinematics in the center-of-mass system,

$$H = \sqrt{\vec{p}^{\,2} + m_1^2} + \sqrt{\vec{p}^{\,2} + m_2^2} + V(\vec{x}) \quad . \tag{1}$$

Applied to the phase-space variables $\vec{p}$ and $\vec{x}$, the operator

$$D = e^{\frac{i}{2}(\ln \lambda)(\vec{p}\vec{x} + \vec{x}\vec{p})} \tag{2}$$

generates the dilatations

$$D\vec{p}D^{-1} = \frac{1}{\lambda}\vec{p} \quad , \qquad D\vec{x}D^{-1} = \lambda\vec{x} \quad . \tag{3}$$

Under these transformations the Hamiltonian (1) behaves like

$$DHD^{-1} = \sqrt{\frac{1}{\lambda^2}\vec{p}^{\,2} + m_1^2} + \sqrt{\frac{1}{\lambda^2}\vec{p}^{\,2} + m_2^2} + V(\lambda\vec{x}) \quad . \tag{4}$$

The virial theorem follows most easily from the first derivative of the dilated Hamiltonian DHD^{-1} w.r.t. $t \equiv \ln\lambda$ at $t = 0$. Expanding in powers of t, we find

$$\sqrt{\frac{1}{\lambda^2}\vec{p}^{\,2} + m^2} = \sqrt{\vec{p}^{\,2} + m^2} - \frac{\vec{p}^{\,2}}{\sqrt{\vec{p}^{\,2} + m^2}}\, t + O(t^2) \tag{5}$$

and

$$V(\lambda\vec{x}) - V(\vec{x}) = t\vec{x}\cdot\vec{\nabla}V(\vec{x}) + O(t^2) \quad . \tag{6}$$

In the following, all expectation values are understood to be taken w.r.t. normalized eigenstates of the Hamiltonian (1), with energy $E \equiv \langle H\rangle$. Then $\langle (DHD^{-1})D\rangle = \langle HD\rangle$ holds since both sides equal $E\langle D\rangle$.

Dividing the difference of the l.h.s. and r.h.s. of this equality by t and performing the limit $t \to 0$, we obtain

$$\begin{aligned}
&\lim_{t\to 0}\frac{1}{t}\langle (DHD^{-1}-H)D\rangle \\
&= \left\langle -\frac{\vec{p}^{\,2}}{\sqrt{\vec{p}^{\,2}+m_1^2}} - \frac{\vec{p}^{\,2}}{\sqrt{\vec{p}^{\,2}+m_2^2}} + \vec{x}\cdot\vec{\nabla}V(\vec{x})\right\rangle = 0 \quad , \qquad (7)
\end{aligned}$$

which is the relativistic virial theorem:

$$\langle \vec{x}\cdot\vec{\nabla}V(\vec{x})\rangle = \left\langle \frac{\vec{p}^{\,2}}{\sqrt{\vec{p}^{\,2}+m_1^2}} + \frac{\vec{p}^{\,2}}{\sqrt{\vec{p}^{\,2}+m_2^2}}\right\rangle \quad . \qquad (8)$$

In the nonrelativistic case it reduces to the well-known form

$$\langle \vec{x}\cdot\vec{\nabla}V(\vec{x})\rangle = \left\langle \frac{\vec{p}^{\,2}}{\mu}\right\rangle \quad , \qquad (9)$$

where $\mu = m_1 m_2/(m_1+m_2)$ is the reduced mass of the two-particle system under consideration. For a central potential $V = V(r)$ the directional derivative $\vec{x}\cdot\vec{\nabla}V(\vec{x})$ is simply $r\frac{d}{dr}V(r)$ [7].

The decomposition

$$\frac{\vec{p}^{\,2}}{\sqrt{\vec{p}^{\,2}+m^2}} = \sqrt{\vec{p}^{\,2}+m^2} - \frac{m^2}{\sqrt{\vec{p}^{\,2}+m^2}} \qquad (10)$$

allows us to use the above theorem (8) in the computation of the eigenvalues of the Hamiltonian (1):

$$\begin{aligned}
E \;\equiv\; \langle H\rangle &= \langle \sqrt{\vec{p}^{\,2}+m_1^2}+\sqrt{\vec{p}^{\,2}+m_2^2}\rangle + \langle V(\vec{x})\rangle \\
&= \langle \vec{x}\cdot\vec{\nabla}V(\vec{x})\rangle + \langle V(\vec{x})\rangle + \left\langle \frac{m_1^2}{\sqrt{\vec{p}^{\,2}+m_1^2}} + \frac{m_2^2}{\sqrt{\vec{p}^{\,2}+m_2^2}}\right\rangle \quad . \qquad (11)
\end{aligned}$$

The last expectation value in the above expression drops out in the ultra-relativistic case $m_1 = m_2 = 0$,

$$E = \langle \vec{x}\cdot\vec{\nabla}V(\vec{x})\rangle + \langle V(\vec{x})\rangle \quad , \qquad (12)$$

whereas it contributes via the virial theorem (9) to $\langle \vec{x}\cdot\vec{\nabla}V\rangle$ in the nonrelativistic case,

$$\begin{aligned}
E &= \langle \vec{x}\cdot\vec{\nabla}V(\vec{x})\rangle + \langle V(\vec{x})\rangle + m_1 + m_2 - \left\langle \frac{\vec{p}^{\,2}}{2\mu}\right\rangle \\
&= m_1 + m_2 + \frac{1}{2}\langle \vec{x}\cdot\vec{\nabla}V(\vec{x})\rangle + \langle V(\vec{x})\rangle \quad . \qquad (13)
\end{aligned}$$

Two main features characterize any realistic "QCD-inspired" inter-quark potential: Its short-distance behaviour is dominated by one-gluon exchange (which gives an approximately Coulomb-like contribution),

$$\lim_{r\to 0} V(r) \simeq -\frac{4}{3}\frac{\alpha_s}{r} \quad , \tag{14}$$

while at large distances it has to provide for confinement,

$$\lim_{r\to\infty} V(r) \simeq ar \quad . \tag{15}$$

The most simple-minded picture is thus represented just by the sum of these two contributions, which is the funnel or Cornell potential [8,9,10]

$$V(r) = -\frac{4}{3}\frac{\alpha_s}{r} + ar \quad . \tag{16}$$

The potential V enters into the expression (11) for the energy of the bound state, however, in a way in which its Coulomb part cancels, $r\frac{d}{dr}V(r) + V(r) = 2ar$. Despite the presence of the Coulomb term in the potential the quarks only feel the linear part. In contrast to that, due to the factor $\frac{1}{2}$ in front of $\langle \vec{x}\cdot\vec{\nabla}V\rangle$ in (13), this cancellation is incomplete in the nonrelativistic version. Consequently, for light masses of the constituents, the nonrelativistic treatment of bound states with a purely linear potential $V_{\rm NR} = \hat{a}r$ is equivalent to the relativistic treatment with the funnel potential (16). The corresponding slopes are related by $\hat{a} = \frac{4}{3}a$. In other words, ignoring in a nonrelativistic computation the Coulomb part of the potential for light particles simulates a relativistic calculation.

There are some further, but less rigorous, hints why the description of bound states by the nonrelativistic Schrödinger formalism might not be complete nonsense.

First of all, according to $|\langle\mathcal{O}\rangle| \le \sqrt{\langle\mathcal{O}^2\rangle}$ valid for any hermitian operator $\mathcal{O}$, the relativistic kinetic energy satisfies $\langle\sqrt{\vec{p}^2+m^2}\rangle \le \sqrt{\langle\vec{p}^2\rangle+m^2}$. From this one finds for the expectation value of H

$$\begin{aligned}\langle H\rangle &= 2\langle\sqrt{\vec{p}^2+m^2}\rangle + \langle V\rangle \le 2\sqrt{\langle\vec{p}^2\rangle+m^2} + \langle V\rangle \\ &= 2\frac{\langle\vec{p}^2\rangle+m^2}{\sqrt{\langle\vec{p}^2\rangle+m^2}} + \langle V\rangle = \left\langle 2\frac{\vec{p}^2+m^2}{\sqrt{\langle\vec{p}^2\rangle+m^2}} + V\right\rangle \quad .\end{aligned} \tag{17}$$

Consequently, the relativistic Hamiltonian is bounded from above by

$$H \le 2\frac{\vec{p}^2+m^2}{\sqrt{\langle\vec{p}^2\rangle+m^2}} + V \quad . \tag{18}$$

The operator on the r.h.s. of this inequality is formally of the same structure as the nonrelativistic Schrödinger Hamiltonian

$$H_{\rm NR} = 2\hat{m} + \frac{\vec{p}^{\,2}}{\hat{m}} + V_{\rm NR} \tag{19}$$

with, however, an effective mass $\hat{m} = \frac{1}{2}\sqrt{\langle\vec{p}^{\,2}\rangle + m^2}$ and the nonrelativistic potential

$$V_{\rm NR} = \frac{2m^2}{\sqrt{\langle\vec{p}^{\,2}\rangle + m^2}} - \sqrt{\langle\vec{p}^{\,2}\rangle + m^2} + V = 2\hat{m} - \frac{\langle\vec{p}^{\,2}\rangle}{\hat{m}} + V \quad . \tag{20}$$

The effective mass $\hat{m}$ as well as the constant in the potential $V_{\rm NR}$ depend on the average momentum $\langle\vec{p}^{\,2}\rangle$ and will thus vary from level to level. The expectation value of the kinetic energy is related by the nonrelativistic virial theorem (9) to $\langle r\frac{d}{dr}V(r)\rangle$. The latter is a constant only for the exceptional case of a logarithmic potential $\propto \ln(r/r_0)$ [11]. Only in this case $\langle\vec{p}^{\,2}\rangle$ is independent of the level of excitation.

Secondly, there exists a certain kind of duality between an ultrarelativistic Hamiltonian with harmonic-oscillator potential and a nonrelativistic Hamiltonian with linear potential [12]: The ultra-relativistic Hamiltonian $H_{\rm UR} = 2\sqrt{\vec{p}^{\,2}} + \kappa r^2$ is converted into the nonrelativistic Hamiltonian $H_{\rm NR} = \vec{p}^{\,2}/m + ar$ by means of the duality transformation $|\vec{p}| \to ar/2$, $r \to 2|\vec{p}|/a$, provided the parameters κ, a, and m are related by $\kappa = a^2/(4m)$. The eigenfunctions in the corresponding wave equations, $H_{\rm UR}\phi(\vec{x}) = E\phi(\vec{x})$ and $H_{\rm NR}\psi(\vec{y}) = E\psi(\vec{y})$, resp., are then connected by the Fourier transformation $\phi(\vec{x}) = \int d^3y\, \exp(i\frac{a}{2}\vec{x}\cdot\vec{y})\,\psi(\vec{y})$.

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