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Relativistic Virial Theorem

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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.

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In nonrelativistic quantum mechanics the so-called virial theorem relates the kinetic energy of a system to the expectation value of the directional derivative of the potential. Unfortunately, this theorem applies only to nonrelativistic kinematics. In this Letter we derive a theorem which may be regarded as the relativistic generalization of this well-known relation. This relativistic virial theorem relates the expectation value of the directional derivative of the potential to the expectation value of an operator which involves the relativistic kinetic energy. It comprises, of course, the nonrelativistic theorem as a special case.

With the relativistic virial theorem at our disposal we are, for instance, able to cast some light on a long-standing puzzle in hadron spectroscopy: The description of hadrons consisting of light quarks by two seemingly different approaches, viz. in terms of the nonrelativistic Schrödinger formalism, on the one hand[1] (for a rather comprehensive list of references, see Refs. 2 and 3), and by a semirelativistic Hamiltonian incorporating relativistic kinematics, on the other hand,[4-7] produces comparably good results.

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

$$H=(\mathbf{p}^2+m_1^2)^{1/2}+(\mathbf{p}^2+m_2^2)^{1/2}+V(\mathbf{x}). \tag{1}$$

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

$$D=e^{(i/2)(\ln\lambda)(\mathbf{p}\cdot\mathbf{x}+\mathbf{x}\cdot\mathbf{p})} \tag{2}$$

generates the dilatations

$$D\mathbf{p}D^{-1}=(1/\lambda)\mathbf{p},\quad D\mathbf{x}D^{-1}=\lambda\mathbf{x}. \tag{3}$$

Under these transformations the Hamiltonian (1) behaves like

$$DHD^{-1}=\left(\frac{1}{\lambda^2}\mathbf{p}^2+m_1^2\right)^{1/2}+\left(\frac{1}{\lambda^2}\mathbf{p}^2+m_2^2\right)^{1/2}+V(\lambda\mathbf{x}). \tag{4}$$

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

$$\left(\frac{1}{\lambda^2}\mathbf{p}^2+m^2\right)^{1/2}=(\mathbf{p}^2+m^2)^{1/2}-\frac{\mathbf{p}^2}{(\mathbf{p}^2+m^2)^{1/2}}t+O(t^2) \tag{5}$$

and

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

In the following, all expectation values are understood to be taken with respect to the normalized eigenstates of the Hamiltonian (1), with an 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 left-hand side and right-hand side of this equality by t and performing the limit

$t \to 0$, we obtain

$$\lim_{t\to 0}\frac{1}{t}\langle (DHD^{-1}-H)D\rangle = \left\langle -\frac{\mathbf{p}^2}{(\mathbf{p}^2+m_1^2)^{1/2}} - \frac{\mathbf{p}^2}{(\mathbf{p}^2+m_2^2)^{1/2}} + \mathbf{x}\cdot\nabla V(\mathbf{x})\right\rangle = 0\,, \tag{7}$$

which is the relativistic virial theorem:

$$\langle \mathbf{x}\cdot\nabla V(\mathbf{x})\rangle = \left\langle \frac{\mathbf{p}^2}{(\mathbf{p}^2+m_1^2)^{1/2}} + \frac{\mathbf{p}^2}{(\mathbf{p}^2+m_2^2)^{1/2}}\right\rangle. \tag{8}$$

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

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

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 $\mathbf{x}\cdot\nabla V(\mathbf{x})$ is simply $r(d/dr)V(r)$.[8]

The decomposition

$$\frac{\mathbf{p}^2}{(\mathbf{p}^2+m^2)^{1/2}} = (\mathbf{p}^2+m^2)^{1/2} - \frac{m^2}{(\mathbf{p}^2+m^2)^{1/2}} \tag{10}$$

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

$$E\equiv\langle H\rangle = \langle (\mathbf{p}^2+m_1^2)^{1/2} + (\mathbf{p}^2+m_2^2)^{1/2}\rangle + \langle V(\mathbf{x})\rangle = \langle \mathbf{x}\cdot\nabla V(\mathbf{x})\rangle + \langle V(\mathbf{x})\rangle + \left\langle \frac{m_1^2}{(\mathbf{p}^2+m_1^2)^{1/2}} + \frac{m_2^2}{(\mathbf{p}^2+m_2^2)^{1/2}}\right\rangle. \tag{11}$$

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

$$E = \langle \mathbf{x}\cdot\nabla V(\mathbf{x})\rangle + \langle V(\mathbf{x})\rangle\,, \tag{12}$$

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

$$E = \langle \mathbf{x}\cdot\nabla V(\mathbf{x})\rangle + \langle V(\mathbf{x})\rangle + m_1 + m_2 - \left\langle \frac{\mathbf{p}^2}{2\mu}\right\rangle = m_1+m_2+\tfrac{1}{2}\langle \mathbf{x}\cdot\nabla V(\mathbf{x})\rangle + \langle V(\mathbf{x})\rangle\,. \tag{13}$$

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

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

while at large distances it has to provide for confinement,

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

The most simple-minded picture is thus represented just by the sum of these two contributions, which is the funnel or Cornell potential,[9-11]

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

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, $r(d/dr)V(r)+V(r)=2ar$. In contrast to that, due to the factor $\frac{1}{2}$ in front of $\langle \mathbf{x}\cdot\nabla V\rangle$ in (13), this cancellation is incomplete in the nonrelativistic version. Consequently, to the extent that the third term on the right-hand side of Eq. (11) may be neglected, the expectation value of the nonrelativistic Hamiltonian with a purely linear potential $V_{\rm nr}=ar$ is of formal resemblance to the expectation value of the relativistic Hamiltonian with the funnel potential (16). The corresponding eigenstates are, of course, different. Nevertheless, the above similarity may lead one astray to treat bound states of light constituents nonrelativistically, by employing only a linear potential.

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

First of all, according to $|\langle \mathcal{O}\rangle| \le \langle \mathcal{O}^2\rangle^{1/2}$ valid for any Hermitian operator $\mathcal{O}$, the relativistic kinetic energy satisfies $\langle (\mathbf{p}^2+m^2)^{1/2}\rangle \le (\langle \mathbf{p}^2\rangle + m^2)^{1/2}$. From this one finds for the expectation value of H (for equal masses $m_1=m_2=m$)

$$\langle H\rangle = 2\langle (\mathbf{p}^2+m^2)^{1/2}\rangle + \langle V\rangle \le 2(\langle \mathbf{p}^2\rangle + m^2)^{1/2} + \langle V\rangle = 2\frac{\langle \mathbf{p}^2\rangle + m^2}{(\langle \mathbf{p}^2\rangle + m^2)^{1/2}} + \langle V\rangle = \left\langle 2\frac{\mathbf{p}^2+m^2}{(\langle \mathbf{p}^2\rangle + m^2)^{1/2}} + V\right\rangle. \tag{17}$$

Consequently, the relativistic energy eigenvalue $E\equiv\langle H\rangle$ is bounded from above by

$$E \le \left\langle 2\frac{\mathbf{p}^2+m^2}{(\langle \mathbf{p}^2\rangle + m^2)^{1/2}} + V\right\rangle. \tag{18}$$

The operator on the right-hand side of this inequality is formally of the same structure as the nonrelativistic Schrödinger Hamiltonian

$$H_{\rm nr} = 2\hat{m} + \frac{\mathbf{p}^2}{\hat{m}} + V_{\rm nr} \tag{19}$$

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

$$V_{\rm nr} = \frac{2m^2}{(\langle \mathbf{p}^2\rangle + m^2)^{1/2}} - (\langle \mathbf{p}^2\rangle + m^2)^{1/2} + V = 2\hat{m} - \frac{\langle \mathbf{p}^2\rangle}{\hat{m}} + V\,. \tag{20}$$

The effective mass $\hat{m}$ as well as the constant in the potential $V_{\rm nr}$ depend on the average momentum $\langle \mathbf{p}^2\rangle$ and

will thus vary from level to level. The expectation value of the kinetic energy is related by the nonrelativistic virial theorem (9) to $\langle r(d/dr)V(r)\rangle$. The latter is a constant only for the exceptional case of a logarithmic potential $\propto \ln(r/r_0)$.[12] Only in this case is $\langle \mathbf{p}^2\rangle$ independent of the level of excitation.

Second, there exists a certain kind of duality between the ultrarelativistic Hamiltonian with a harmonic-oscillator potential and a nonrelativistic Hamiltonian with a linear potential:[13] The ultrarelativistic Hamiltonian $H_{\rm ur}=2(\mathbf{p}^2)^{1/2}+\kappa r^2$ is converted into the nonrelativistic Hamiltonian $H_{\rm nr}=\mathbf{p}^2/m+ar$ by means of the duality transformation $|\mathbf{p}|\rightarrow ar/2$, $r\rightarrow 2|\mathbf{p}|/a$, provided the parameters κ, a, and m are related by $\kappa=a^2/4m$. The eigenfunctions in the corresponding wave equations, $H_{\rm ur}\phi(\mathbf{x})=E\phi(\mathbf{x})$ and $H_{\rm nr}\psi(\mathbf{y})=E\psi(\mathbf{y})$, respectively, are then connected by the Fourier transformation $\phi(\mathbf{x})=\int d^3y \exp[i(a/2)\mathbf{x}\cdot\mathbf{y}]\psi(\mathbf{y})$.

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