Virial theorems for relativistic spin-$\frac{1}{2}$ and spin-0 particles

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We derive virial theorems for relativistic particles which obey the Dirac or the Klein-Gordon equation and are bound in scalar- and/or vector-type potentials.

I. INTRODUCTION

The quantum-mechanical virial theorem for a nonrelativistic particle, bound in a local potential $V(\vec{r})$,

$$[\hat{T}+V(\vec{r})]\varphi_i(\vec{r})=E_i\varphi_i(\vec{r}) \quad , \tag{1}$$

says that for all states φ_i the following relation holds[1]:

$$\langle i|\hat{T}|i\rangle=\tfrac{1}{2}\langle i|\vec{r}\cdot\vec{\nabla}V|i\rangle \quad . \tag{2}$$

If the potential follows a power law $V(\vec{r})=ar^n$, one has the familiar forms

$$\langle i|\hat{T}|i\rangle=\frac{n}{2}\langle i|V|i\rangle \quad , \tag{3a}$$

$$E_i=\tfrac{1}{2}(n+2)\langle i|V|i\rangle \quad . \tag{3b}$$

Since over the last few years there has been a growing interest in the spectra of relativistic quarks bound in various types of confinement potentials,[2–4] it might be useful for the modeling of such confinement potentials to have the corresponding relativistic virial theorem at hand. Strangely enough, we were not able to find it in the current literature on relativisitc quantum mechanics. In this Brief Report, we shall derive the virial theorems for both Dirac and Klein-Gordon particles. We shall hereby use the principle of scale invariance, which is often used to derive the classical nonrelativistic virial theorem,[5] and briefly illustrate it first for deriving Eq. (2) which is usually obtained by requiring that the time derivative of $\langle\vec{r}\cdot\vec{p}\rangle$ vanishes for a bound state.[1]

The Schrödinger equation (1) can be viewed as a result of a variational calculation in which the expectation value $\langle\varphi_i|\hat{T}+V|\varphi_i\rangle$ is minimized with respect to variations of the wave function $\varphi_i(\vec{r})$ which conserve its norm and do not change its symmetries and additional quantum numbers (angular momentum, number of radial nodes, parity, etc.). One particular variation which has these properties is the scale transformation

$$\varphi_i(\vec{r})\rightarrow\varphi_i^{(\lambda)}(\vec{r})=\lambda^{3/2}\varphi_i(\lambda\vec{r}) \quad . \tag{4}$$

After this transformation, the expectation value of $\hat{T}+V$ becomes, with a simple substitution of variables,

$$E_i(\lambda)=\lambda^2\langle\varphi_i|\hat{T}|\varphi_i\rangle+\langle\varphi_i|V(\vec{r}/\lambda)|\varphi_i\rangle \quad ,$$

where φ_i are again the unscaled wave functions. Requiring $E_i(\lambda)$ to be stationary at $\lambda=1$, we write

$$\left.\frac{\partial E_i}{\partial\lambda}\right|_{\lambda=1}=\left(2\lambda\langle i|\hat{T}|i\rangle-\frac{1}{\lambda}\langle i|\vec{r}\cdot\vec{\nabla}_r V(\vec{r}/\lambda)|i\rangle\right)_{\lambda=1}=0 \quad ,$$

from which the virial theorem Eq. (2) immediately follows. The condition for E_i to have a minimum at $\lambda=1$ becomes, for potentials $V(\vec{r})=Kr^n$,

$$\left.\frac{\partial^2E_i}{\partial\lambda^2}\right|_{\lambda=1}=2\langle i|\hat{T}|i\rangle+n(n+1)\langle i|V|i\rangle>0 \quad ,$$

or, with Eq. (3.a),

$$n(n+2)\langle i|V|i\rangle>0 \quad .$$

For potentials $V(r)<0$ this inequality requires $0>n>-2$ which recalls the well-known fact that, for $n<-2$, a bound state with finite energy cannot exist.[6] [For $n=-2$, we find $E_i=0$ from Eq. (3b).]

The present derivation of the virial theorem makes it very easy to study the influence of a weak *constant* external magnetic field $\vec{B}_0$. Starting from the Pauli equation with the vector potential $\vec{A}=\frac{1}{2}(\vec{B}_0\times\vec{r})$ and neglecting the terms in $\vec{A}^2$, one obtains the familiar form for the energy

$$E_i=\langle i|\hat{T}|i\rangle+\langle i|V|i\rangle-\langle i|\vec{\mu}\cdot\vec{B}_0|i\rangle \quad .$$

Now, since the magnetic-moment operator

$$\vec{\mu}=\frac{e\hbar}{2mc}[-i(\vec{r}\times\vec{\nabla})+\vec{\sigma}] \tag{5}$$

does *not* change under the scale transformation Eq. (4), the Zeeman term does not contribute to $\partial E_i/\partial\lambda$ and thus the Eqs. (2) and (3a) for the nonrelativistic virial theorem remain unaltered (up to some neglected $\vec{A}^2$ terms). In Eq. (3b), of course, the magnetic interaction energy $-\langle i|\vec{\mu}\cdot\vec{B}_0|i\rangle$ has to be added on the right-hand side.

II. DIRAC PARTICLES

Consider now a spin-$\frac{1}{2}$ particle obeying the Dirac equation. In the relativistic theory, we must differentiate between two types of potentials which behave like scalars or four-vectors, respectively, under Lorentz transformations. The vector type is represented by the electromagnetic four-vector potential $A^{\mu}=(W,\vec{A})$. A scalar-type potential is, e.g., used in relativisitic phenomenological quark models[2–4] as a confinement potential; a vector potential cannot confine simultaneously quarks and antiquarks.[7]

For the sake of generality, we assume both types of potentials to be present; however, we shall keep only the zeroth component $W(\vec{r})$ of the vector potential, in order not to make the presentation too clumsy, and discuss the effect of a magnetic potential $\vec{A}$ at the end of this section. Denoting the scalar potential[8] by $V(\vec{r})$, the Dirac equation then is

$$\{c\vec{\alpha}\cdot\vec{p}+W(\vec{r})+\beta[V(\vec{r})+mc^2]\}\Psi=E\Psi \tag{6}$$

in the usual notation. (We omit henceforth the indices for the quantum numbers of the bound states.) We write the Dirac spinor Ψ in the usual way,

$$\Psi=\begin{pmatrix}\psi_A\\ \psi_B\end{pmatrix},\quad \int\Psi^\dagger\Psi\, d^3r=1\ ,$$

and define the norms of the two components:

$$\int\psi_A^\dagger\psi_A d^3r=N_A,\quad \int\psi_B^\dagger\psi_B d^3r=N_B,\quad N_A+N_B=1\ .$$

The scaling method described above can be applied in a straightforward way. We scale the entire spinor $\Psi(\vec{r})$, i.e., all four components simultaneously, as in Eq. (4):

$$\Psi(\vec{r})\to\lambda^{3/2}\Psi(\lambda\vec{r})\ .$$

Although the components ψ_A and ψ_B are not independent, the variational principle still requires E to be minimal at $\lambda=1$, if one starts from the exact solution of Eq. (6). Proceeding as in the nonrelativistic case, we find now the virial theorem for Dirac particles:

$$\langle c\vec{\alpha}\cdot\vec{p}\rangle=\langle\hat{T}\rangle=\langle\beta\vec{r}\cdot\vec{\nabla}V\rangle+\langle\vec{r}\cdot\vec{\nabla}W\rangle\ . \tag{7}$$

In contrast to the nonrelativistic case Eq. (2), the factor 2 is missing due to the linear dependence of the Dirac kinetic energy operator on $\vec{p}=-i\hbar\vec{\nabla}$.

Assuming the potentials to follow power laws

$$V(\vec{r})=Kr^n,\quad W(\vec{r})=Qr^p\ , \tag{8}$$

we have

$$\langle\hat{T}\rangle=n\langle\beta V\rangle+p\langle W\rangle\ . \tag{9}$$

Note that in Eqs. (7) and (9) and below, the simple angular brackets are always expectation values between the full spinors $\Psi^\dagger$ and Ψ. Eliminating the kinetic energy from Eq. (9) and the expression for the total energy

$$E=\langle\hat{T}\rangle+\langle W\rangle+\langle\beta V\rangle+mc^2(N_A-N_B)\ , \tag{10}$$

we obtain

$$E=(p+1)\langle W\rangle+(n+1)\langle\beta V\rangle+mc^2(N_A-N_B)\ . \tag{11}$$

The quantity (N_A-N_B) depends in general on the quantum numbers of the state and cannot be expressed simply in terms of E, n, and p [except for $n=p=-1$ and for $V(\vec{r})=W(\vec{r})$, see below].

For the stability condition,

$$\left.\frac{\partial^2E}{\partial\lambda^2}\right|_{\lambda=1}>0\ ,$$

we find

$$p(p+1)\langle W\rangle+n(n+1)\langle\beta V\rangle>0\ . \tag{12}$$

In general cases with a scalar potential $V\neq0$, we cannot draw any conclusions from this inequality, since the sign of

$$\langle\beta V\rangle=\int d^3r\, V(\vec{r})(\psi_A^\dagger\psi_A-\psi_B^\dagger\psi_B)$$

is not known in general. In purely vector-type attractive potentials ($V\equiv0$) with $p<0$, we find $0>p>-1$ from Eq. (12). Thus, the Coulomb potential ($p=-1$) plays a similar role here as a $1/r^2$ potential in the Schrödinger case, although finite binding energies do exist here, as we all know from the hydrogen atom. If we put $n=p=-1$ in Eq. (11), we find the interesting relation

$$E=mc^2(N_A-N_B)\ , \tag{13}$$

i.e., the kinetic and potential energies cancel in Eq. (10) and the binding energies live from the difference in the norms of ψ_A and ψ_B alone.[9] The Coulomb potential is peculiar also in that E is completely independent of the above scale transformation or any variations which leave the norms of ψ_A and ψ_B unchanged. We also learn immediately from Eq. (13) that *massless* Dirac particles cannot be bound by a $1/r$ potential of either vector or scalar type.

We may also write down "partial virial theorems" for the expectation values of the potential with respect to either ψ_A or ψ_B alone. We shall briefly demonstrate this for a pure scalar potential $V=Kr^n$ ($W\equiv0$). Decomposing the Dirac equation into two coupled equations for ψ_A and ψ_B and eliminating the latter with

$$\psi_B=\frac{c}{E+mc^2+V}(\vec{\sigma}\cdot\vec{p})\psi_A\ , \tag{14}$$

we get the equation

$$\left[(\vec{\sigma}\cdot\vec{p})\frac{c^2}{E+mc^2+V}(\vec{\sigma}\cdot\vec{p}) + V(\vec{r}) + mc^2\right]\psi_A = E\psi_A \ . \quad (15)$$

Introducing the symbol $\langle\ \rangle_A$ for normalized expectation values with respect to ψ_A, i.e.,

$$\langle V\rangle_A = \frac{1}{N_A}\int \psi_A^\dagger V\psi_A d^3r \ , \quad (16)$$

etc., we can find the energy as a solution of the implicit equation

$$E = \langle\hat{T}_+\rangle_A + \langle V\rangle_A + mc^2 \ , \quad (17)$$

where $\hat{T}_+$ is the first operator in the square brackets of Eq. (15) which contains E in the denominator. We now apply the scale transformation Eq. (4) to ψ_A and require E in Eq. (17) to be stationary at $\lambda = 1$ again. After some algebraic manipulations and using Eq. (14) we find

$$(n+2)\langle\hat{T}_+\rangle_A = n\langle V\rangle_A - n(E+mc^2)(N_B/N_A) \ . \quad (18)$$

Eliminating $\langle\hat{T}_+\rangle_A$ from Eqs. (17) and (18) we obtain

$$\langle V\rangle_A = \frac{1}{(2n+2)}\left[(n+2)(E-mc^2) - n(E+mc^2)\frac{N_B}{N_A}\right] \quad (19)$$

$$(n \neq -1) \ .$$

[For $n=-1$ one gets Eq. (13) back again.] We repeat now the same procedure with exchanged roles of ψ_A and ψ_B, parallel to Eqs. (14)–(19), to find

$$\langle V\rangle_B = \frac{1}{(2n+2)}\left[-(n+2)(E+mc^2) + n(E-mc^2)\frac{N_A}{N_B}\right] \quad (20)$$

$$(n \neq -1)$$

where $\langle V\rangle_B$ is defined analogously to Eq. (16) in terms of ψ_B. From Eqs. (19) and (20) we can obtain Eq. (11) back (with $W \equiv 0$), noticing that

$$\langle\beta V\rangle = N_A\langle V\rangle_A - N_B\langle V\rangle_B \ .$$

Although $\langle V\rangle_A$ and $\langle V\rangle_B$ individually have little physical meaning, Eqs. (19) and (20) contain more information than Eq. (11). As an illustration for an application, we calculate the mean-square radius of a Dirac particle in a scalar potential with $n=2$:

$$V(r) = Kr^2 \ .$$

Writing

$$\langle r^2\rangle = N_A\langle r^2\rangle_A + N_B\langle r^2\rangle_B \ ,$$

we can use the above results for $\langle V\rangle_A$ and $\langle V\rangle_B$ to find

$$\langle r^2\rangle = [E(N_A - N_B) - mc^2]/K \ .$$

We finally mention the particular combination of identical scalar and vector potentials:

$$V(\vec{r}) \equiv W(\vec{r}) = \tfrac{1}{2}U(\vec{r}) \ . \quad (21)$$

Although this hardly corresponds to a physical situation, it has the nice feature[3] that the Dirac equation (6) then reduces to the equation

$$\left(\frac{c^2}{E+mc^2}\vec{p}^2 + U(\vec{r})\right)\psi_A = (E-mc^2)\psi_A \quad (22)$$

which can be solved analytically whenever this is possible for the Schrödinger equation with the same potential. Assuming $U(\vec{r}) = Kr^n$, we find in this case

$$\langle U\rangle_A = \frac{2}{n+2}(E-mc^2) \quad (n \neq -2) \quad (23)$$

which looks like the nonrelativistic virial theorem but does not contradict Eq. (11). Moreover, we can in this case express the difference $(N_B - N_A)$ in terms of E, n, and the mass:

$$N_A - N_B = \frac{E+(n+1)mc^2}{(n+1)E+mc^2} \ .$$

If we add an external magnetic field $\vec{B} = \vec{\nabla}\times\vec{A}$, we have to make the "minimal substitution" $\vec{p} \to \vec{p} - (e/c)\vec{A}$ in the Dirac equaton (6), which leads to the interaction energy

$$\Delta E = -e\langle\vec{\alpha}\cdot\vec{A}\rangle = -\frac{1}{c}\langle\vec{j}\cdot\vec{A}\rangle \ ,$$

where $\vec{j} = ec\psi^\dagger\vec{\alpha}\psi$ is the Dirac current. This leads to an additional term $-(1/c)\langle\vec{j}\cdot(\vec{r}\cdot\vec{\nabla})\vec{A}\rangle$ on the right-hand side of Eq. (7). For a *homogeneous* magnetic field $\vec{B}_0$, $\vec{A} = \frac{1}{2}(\vec{B}_0\times\vec{r})$ is linear in $\vec{r}$ and then the correction term is identical to the Zeeman term,

$$-\frac{1}{c}\langle\vec{j}\cdot(\vec{r}\cdot\vec{\nabla})\vec{A}\rangle = -\frac{1}{c}\langle\vec{j}\cdot\vec{A}\rangle = -\langle\vec{\mu}\cdot\vec{B}_0\rangle$$

with the relativistic form of the magnetic moment

$$\vec{\mu} = \frac{1}{2c}\int(\vec{r}\times\vec{j})d^3r \ . \quad (24)$$

Thus, in contrast to the nonrelativistic case again, the Zeeman energy $-\langle\vec{\mu}\cdot\vec{B}_0\rangle$ does appear in the relativistic virial theorem for $\langle\hat{T}\rangle$, Eq. (7) and, with a factor 2, in the corresponding Eq. (11) for the energy.

III. KLEIN-GORDON PARTICLES

The case of spin-0 particles is quickly dealt with. We start from the linearized form of the Klein-Gordon equation,[1] including again a scalar and a vector potential:

$$\left[\frac{\vec{p}^2}{2m}(\tau_3+i\tau_2) + W(\vec{r}) + \tau_3[V(\vec{r}) + mc^2]\right]\Phi = E\Phi \quad . \tag{25}$$

Here τ_2 and τ_3 are identical with the Pauli matrices, and the wave function has two *scalar* components ψ_A and ψ_B,

$$\Phi = \begin{bmatrix}\psi_A\\ \psi_B\end{bmatrix} \quad ,$$

and shall be normalized as Ψ above. Since the kinetic energy operator in Eq. (25) is quadratic in $\vec{p}$, we get the factors here as in the nonrelativistic virial theorem:

$$\left\langle \frac{\vec{p}^2}{2m}(\tau_3+i\tau_2)\right\rangle = \langle \hat{T}\rangle = \tfrac{1}{2}\langle \vec{r}\cdot\vec{\nabla} W\rangle + \tfrac{1}{2}\langle \tau_3\vec{r}\cdot\vec{\nabla} V\rangle \quad , \tag{26}$$

or, with the forms Eq. (8) of the potentials,

$$E = \tfrac{1}{2}(p+2)\langle W\rangle + \tfrac{1}{2}(n+2)\langle \tau_3 V\rangle + mc^2(N_A - N_B) \quad . \tag{27}$$

The relation (13) arises here in the case $n = p = -2$. The inclusion of a magnetic field is here also analogous to the nonrelativistic case.

Note added in proof: An independent study of the virial theorem for the Dirac H atom, following the classical derivation,[1] was published a few months ago by E. H. de Groot, Am. J. Phys. 50, 1141 (1982).

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[1]See, e.g., A. S. Davydov, in *Quantum Mechanics,* translated and edited by D. ter Haar (Pergamon, New York, 1965).

[2]T. DeGrand *et al.,* Phys. Rev. D 12, 2060 (1975); V. Vento *et al.,* Nucl. Phys. A345, 413 (1980).

[3]G. B. Smith and L. J. Tassie, Ann. Phys. (N.Y.) 65, 352 (1971); P. Leal Ferreira, I. A. Helayel, and N. Zagury, Nuovo Cimento 55A, 215 (1980).

[4]R. Tegen, R. Brockmann, and W. Weise, Z. Phys. A 307, 339 (1982).

[5]See, e.g., L. D. Landau and E. M. Lifshitz, *Mechanics,* Course of Theoretical Physics, Vol. 1, 3rd ed. (Pergamon, Oxford, 1976), Sec. 10. For a discussion of the classical relativistic virial theorem in the Coulomb potential, see Landau and Lifshitz, *The Classical Theory of Fields,* Course of Theoretical Physics, Vol. 2, 4th ed. (Pergamon, Oxford, 1975), Sec. 34.

[6]For an explicit discussion of the case $n = -2$, see L. D. Landau and E. M. Lifshitz, *Quantum Mechanics—Nonrelativistic Theory,* Course of Theoretical Physics, Vol. 3, 3rd ed. (Pergamon, Oxford, 1977), Sec. 35.

[7]This is a consequence of the Klein paradox; see O. Klein, Z. Phys. 53, 157 (1929).

[8]In the context of quark-model phenomenology, the sum $V(\vec{r}) + mc^2$ may be interpreted as a variable quark mass $M(\vec{r})c^2$ which can be viewed as a result of chiral-symmetry breaking; see R. Brockmann, W. Weise, and E. Werner, Phys. Lett. 122B, 201 (1983).

[9]The pedagogically minded reader may amuse himself checking Eq. (13) with the known relativistic wave functions of the Coulomb potential, as given, e.g., in H. Bethe and E. Salpeter, Handb. Phys. 35, 88 (1957).