Relativistic Stationary Schrödinger Equation for Many Particle System and Its Applications

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ABSTRACT

Basing on the fundamental symmetry that the space-time inversion is equavalent to particle-antiparticle transformation, a relativistic modification on the stationary Schrödinger equation for many-particle system is made. The eigenvalue in the center of mass system is no longer equal to the negative of binding energy simply. The possible applications in various fields (e.g. the model of quarkonium) are discussed.

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As is well known in quantum mechanics, for a system composed of two particles with mass m_1 and m_2 and interaction potential $V(|\vec{r_1}-\vec{r_2}|)$, ($\vec{r_1}$ and $\vec{r_2}$ being the coordinates in laboratory (L) system), after introducing the coordinate of center of mass (CM) $\vec{R}=\frac{1}{M}(m_1\vec{r_1}+m_2\vec{r_2})$, $(M=m_1+m_2)$, and relative coordinate $\vec{r}=\vec{r_2}-\vec{r_1}$, one easily obtain the stationary Schrödinger equation

$$[-\frac{\hbar^2}{2\mu}\nabla_{\vec{r}}^2+V(\vec{r})]\psi(\vec{r})=\epsilon\psi(\vec{r}) \tag{1}$$

with reduced mass $\mu=m_1m_2/M$ and eigenvalue

$$\epsilon=E-\frac{P^2}{2M}-Mc^2 \tag{2}$$

where E is the total energy of system in L system and $P=|\vec{P}|$ is the momentum of CM. When $P=0$, $\epsilon=-B<0$, B is called as the binding energy of system.

Usually, it is said that the above "nonrelativistic approximation" is good for the case of $P^2/(2M)$ being small. However, this is doubtful. One can always set the laboratory into motion to render P arbitrary large. Then the accuracy of calculation in CM system would rely on the motion of external world ! Does it respect to the "principle of relativity" in special relativity (SR) ? The reason why one can not isolate his calculation from the external world is the following. The summation of ϵ with $P^2/(2M)$ is made along a straight line in Eq.(2) whereas the correct relation in SR is that of a right triangle:

$$E^2=P^2c^2+(Mc^2-B)^2 \tag{3}$$

Hence, the statement that "the total energy E is equal to the sum of kinetic energy $(P^2/2M)$ of CM and the internal energy (Mc^2-B)" is not rigorous. One should say that "E is equal to the square root of the sum of square of kinetic energy (Pc) of CM and that of internal energy ". Now the problem is "how to modify the Eq.(1) for meeting the requirement of Eq.(3) ?"

It is said in ancient China that "to gain new insights through restudying old material". Let us restudy an alternative derivation of Klein-Gordon (KG) equation. Consider a spinless particle with rest mass m_0 being in free motion. Then its wave function $\theta(\vec{x},t)$ is described by a "nonrelativistic quantum equation":

$$i\hbar\frac{\partial}{\partial t}\theta(\vec{x},t)=m_0c_1^2\theta(\vec{x},t)-\frac{\hbar^2}{2m_0}\nabla^2\theta(\vec{x},t) \tag{4}$$

Here, we add a term of rest energy $m_0c_1^2$ with c_1 being merely a (unfixed yet) constant with dimension of velocity. The next crucial step is assuming that inside a particle state θ, there is always a hiding antiparticle state $\chi(\vec{x},t)$. θ and χ are coupled together via motion. Instead of Eq.(4), we should have a simultaneous equation as follows:

$$\begin{cases} i\hbar\frac{\partial}{\partial t}\theta=m_0c_1^2\theta-\frac{\hbar^2}{2m_0}\nabla^2\theta-\frac{\hbar^2}{2m_0}\nabla^2\chi \\ i\hbar\frac{\partial}{\partial t}\chi=-m_0c_1^2\chi+\frac{\hbar^2}{2m_0}\nabla^2\chi+\frac{\hbar^2}{2m_0}\nabla^2\theta \end{cases} \tag{5}$$

The guiding rule for establishing the Eq.(5) is a basic symmetry. It is invariant under the space-time inversion $\vec{x} \to -\vec{x}$, $t \to -t$ and transformation:

$$\chi(\vec{x}, t) = \theta(-\vec{x}, -t) \tag{6}$$

For solving Eq.(5) in general, we use the ansatz

$$\begin{cases} \theta = (\phi + i\frac{\hbar}{m_0 c_1^2}\dot{\phi}) \\ \chi = (\phi - i\frac{\hbar}{m_0 c_1^2}\dot{\phi}) \end{cases} \tag{7}$$

and obtain the K-G equation

$$(\frac{1}{c_1^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \frac{m_0^2 c_1^2}{\hbar^2})\phi(\vec{x}, t) = 0 \tag{8}$$

Its plane wave solution

$$\phi(\vec{x}, t) = exp[i(\vec{p} \cdot \vec{x} - Et)/\hbar] \tag{9}$$

leads directly to

$$E^2 = \vec{p}^2 c_1^2 + m_0^2 c_1^4 \tag{10}$$

For clarifying the meaning of c_1, we look at the velocity (v) of particle which is equal to the group velocity (v_g) of de'Broglie wave:

$$v = v_g = \frac{d\omega}{dk} = \frac{dE}{dp} = pc_1^2/E, \quad (p = |\vec{p}|) \tag{11}$$

where the quantum relations $E = \hbar\omega$ and $p = hk$ have been used.

The inertial mass is defined as

$$m = \frac{p}{v} = p/(\frac{dE}{dp}) = \frac{1}{2}\frac{d}{dE}\vec{p}^2 \tag{12}$$

Combining Eqs.(10)-(12), we arrive at

$$E = mc_1^2 \tag{13}$$

$$m = m_0/\sqrt{1 - \frac{v^2}{c_1^2}} \tag{14}$$

as expected. But here c has the meaning as the limiting speed of particle, its value is obtained from the measurement on the π meson beam and is coinciding with the speed of light, c:

$$c_1 = c = 3 \times 10^{10}\text{cm/sec} \tag{15}$$

In the above derivation of K-G equation (a reversed version of that in Ref.[1]), we start from $E|_{v=0} = m_0 c_1^2$ and get eventually the mass energy relation $E = mc_1^2$. The proof bears some resemblance to the "inductive method" in mathematics. However, the important thing is injecting into the proof a "relativistic principle", i.e., the basic symmetry (6), which plays the role of "hormone" for activation of mass from m_0 into m.

The symmetry (6) is discussed generally as a statement that "the space-time inversion is equavalent to particle-antiparticle transformation" in Refs. [2-3]. In our opinion, it is a natrual postulate after we learn carefully from the development of physics since the discovery of parity violation [4,5] and the observation of Schwinger et al. [6,7].

We are now in a position to generalize the above derivation to two particle case as in Eq.(1). Denoting $\theta = \theta(\vec{r_1}, \vec{r_2}, t)$ and $\chi = \chi(\vec{r_1}, \vec{r_2}, t)$ the particle and corresponding "antiparticle" state again, then instead of Eq.(5), we can write down the following simultaneous equation:

$$\begin{cases} i\hbar\frac{\partial\theta}{\partial t} = Mc^2\theta - (\frac{\hbar^2}{2m_1}\nabla^2_{\vec{r_1}} + \frac{\hbar^2}{2m_2}\nabla^2_{\vec{r_2}})(\theta+\chi) + V(|\vec{r_1} - \vec{r_2}|)(\theta+\chi) \\ i\hbar\frac{\partial\chi}{\partial t} = -Mc^2\chi + (\frac{\hbar^2}{2m_1}\nabla^2_{\vec{r_1}} + \frac{\hbar^2}{2m_2}\nabla^2_{\vec{r_2}})(\theta+\chi) - V(|\vec{r_1} - \vec{r_2}|)(\theta+\chi) \end{cases} \tag{16}$$

which still respect to the symmetry:

$$\chi(\vec{r_1}, \vec{r_2}, t) = \theta(-\vec{r_1}, -\vec{r_2}, -t) \tag{17}$$

As Eq.(7), we set

$$\theta = \Phi + i\frac{\hbar}{Mc^2}\dot{\Phi}, \quad \chi = \Phi - i\frac{\hbar}{Mc^2}\dot{\Phi} \tag{18}$$

with $\Phi(\vec{r_1}, \vec{r_2}, t) \to \Phi(\vec{R}, \vec{r}, t)$ obeying the equation:

$$\ddot{\Phi} - c^2\nabla^2_{\vec{R}}\Phi - c^2\frac{M}{\mu}\nabla^2_{\vec{r}}\Phi + \frac{1}{\hbar^2}(M^2c^4 + 2VMc^2)\Phi = 0 \tag{19}$$

Factorizing the solution as

$$\Phi(\vec{R}, \vec{r}, t) = e^{i\vec{P}\cdot\vec{R}/\hbar}e^{-iEt/\hbar}\psi(\vec{r}) \tag{20}$$

and substituting it into Eq.(19), we arrive at

$$\begin{cases} [-\frac{\hbar^2}{2\mu}\nabla^2_{\vec{r}} + V(r)]\psi(\vec{r}) = \epsilon\psi(\vec{r}) \\ \epsilon = \frac{1}{2Mc^2}(E^2 - M^2c^4 - P^2c^2) \end{cases} \tag{21}$$

Note that the eigenvalue $\epsilon \neq E - Mc^2$ even when $P = 0$. Comparing Eq.(8) with Eq.(3), we find that the accurate relation between the binding energy B and ϵ reads

$$B = Mc^2[1 - (1 + \frac{2\epsilon}{Mc^2})^{1/2}] \tag{22}$$

Only when $\frac{\epsilon}{Mc^2} << 1$, can one recover the nonrelativistic approximation:

$$B \simeq -\epsilon \tag{23}$$

In general case, one should use Eq.(22) or its equavalent (for $P = 0$):

$$E|_{P=0} = [2Mc^2\epsilon + M^2c^4]^{1/2} \tag{24}$$

It is easy to generalize the above consideration to many particle ($n \geq 3$) case. Denote the coordinates of ith particle with rest mass m_i are $\vec{r'}_i$ and $\vec{r}_i$ in L system and CM system respectively. The coordinate of CM reads $\vec{R} = \sum_{i=1}^{n} \frac{1}{M} m_i \vec{r'}_i$, ($M = \sum_{i=1}^{n} m_i$), while $\vec{r}_i = \vec{r'}_i - \vec{R}$ obeys the constraint:

$$\sum_{i=1}^{n} m_i \vec{r}_i = 0 \tag{25}$$

Direct calculation leads to

$$\sum_{i=1}^{n} \frac{1}{m_i} \nabla^2_{\vec{r'}_i} = \frac{1}{M} \nabla^2_{\vec{R}} + \sum_{i=1}^{n} \frac{1}{m_i} \nabla^2_{\vec{r}_i} - \frac{1}{M} (\sum_{i=1}^{n} \nabla_{\vec{r}_i}) \cdot (\sum_{j=1}^{n} \nabla_{\vec{r}_j}) \tag{26}$$

The third term in RHS can be discarded because in CM system the total momentum equals to zero in stationary state. Denoting $\theta = \theta(\vec{r'}_1, \vec{r'}_2, \cdots, \vec{r'}_n)$, $\chi = \chi(\vec{r'}_1, \vec{r'}_2, \cdots, \vec{r'}_n)$ and introducing again the wave function

$$\Phi(\vec{R}, \vec{r}_i, t) == e^{i\vec{P}\cdot\vec{R}/\hbar} e^{-iEt/\hbar} \psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_n) \tag{27}$$

we find

$$\begin{cases} [-\frac{\hbar^2}{2} \sum_{i=1}^{n} \frac{1}{m_i} \nabla^2_{\vec{r}_i} + \sum_{i<j}^{n} V_{ij}(r_{ij})]\psi = \epsilon\psi \\ \epsilon = \frac{1}{2Mc^2}(E^2 - M^2c^4 - P^2c^2) \end{cases} \tag{28}$$

Similar to Eq.(21). However, only $(n-1)$ coordinates in $\vec{r}_i$ are independent due to the constraint (25).

Some remarks are in order:

1. There is something unreasonable in previous stationary Schrödinger equation (1). The eigenvalue ϵ may fall downward without lower bound. This situation does occur for a singular potential like $V(r) \sim \frac{-1}{r^2}$ (see Refs.[8-9]). Now Eq.(21) has no this kind of worry. There is a minimum value for ϵ: $\epsilon_{\text{min}} = -\frac{1}{2}Mc^2$, or $E_{\text{min}} = 0$. Therefore, the solution of Eq.(21) may be viewed as a variational problem and a lower bound exists for any variational procedure.

2. Let us compare Eq.(21) with Dirac equation. For an electron with mass $m_e = m$ moving in the Coulomb field $V(r) = -Ze^2/(4\pi r)$ of neucleus with mass $m_N \to \infty$, the total energy of electron reads [10]:

$$E_{\text{D}} = mc^2 \{1 + \frac{Z^2\alpha^2}{[\sqrt{(j+1/2)^2 - Z^2\alpha^2} + n']^2}\}^{-1/2} \tag{29}$$

with $\alpha = \frac{e^2}{4\pi\hbar c} \simeq \frac{1}{137}$, $j = \frac{1}{2}, \frac{3}{2}, \cdots$, $n' = 0, 1, 2, \cdots$. In terms of the principal quantum number $n = n' + (j + \frac{1}{2})$, one has

$$E_{\text{D}} = mc^2[1 - \frac{1}{2}\frac{(Z\alpha)^2}{n^2} - \frac{1}{2}\frac{(Z\alpha)^4}{n^3}(\frac{1}{j+1/2} - \frac{3}{4n}) - \cdots] \tag{30}$$

For comparision, the rest energy of neucleus $m_{\text{N}}c^2$ must be substracted from the E derived from Eq.(24). Denote

$$E_{\text{S}} \equiv E - m_{\text{N}}c^2 = c^2(m + m_N)[1 + \frac{2\epsilon}{(m + m_{\text{N}})c^2}]^{1/2} - m_{\text{N}}c^2 \tag{31}$$

where ϵ is well known as

$$\epsilon = -\mu c^2 \frac{Z^2\alpha^2}{2n^2}, \quad (n = 1, 2, \cdots)$$

$$E_{\rm S} = mc^2[1 - \frac{1}{2}\frac{m_N}{(m+m_N)}(\frac{Z\alpha}{n})^2 - \frac{1}{8}\frac{mm_N^2}{(m+m_N)^3}(\frac{Z\alpha}{n})^4 - \cdots] \tag{32}$$

The difference between (30) and (32) is stemming from two reasons. In Dirac equation the spin of electron is taken into account whereas in Eq.(21) the finiteness of neucleas mass is important. However, both equations are relativistic because the basic symmetry (6) is respected (see Refs.[2-3]).
3. Being an improvement to Eq.(1), Eq.(21) or (28) brings some modification on many problems in stationary states. Roughly speaking, for binding state problem, the modification is very small in atomic physics ($< 10^{-5}$), it accounts for 10^{-3} in nuclear physics and may reach 10^{-2} in particle physics. For the high energy scattering problem, this modification might be also important.
4. For concreteness, let us have a quick look at the potential model of heavy quarkonium, $Q\bar{Q}$. Assume that the potential between Q and $\bar{Q}$ is of the linear type, $V(r) = ar$, with constant a being independent of quark mass m. For S states, the stationary equation is solved analytically with eigenvalue

$$\epsilon_n = \lambda_n(\frac{a^2}{2\mu})^{1/3}, \quad (n = 1, 2, \cdots) \tag{33}$$

λ_n being the zeros of Airy function [11]. So the energy (mass) of $Q\bar{Q}$ reads from Eq.(24):

$$E_n = 4\mu[1 + \frac{\lambda_n}{2}(\frac{a^2}{2\mu^4})^{1/3}]^{1/2} \tag{34}$$

with $\mu = \frac{m}{2} = \frac{M}{4}$. On the other hand, the previous equation (1) with (2) yields

$$E_n^{'} = 4\mu^{'} + \lambda_n(\frac{a'^2}{2\mu^{'}})^{1/3} \tag{35}$$

Table 1 is a comparision between the measured energy $E_n^{\rm exp}$ of S states in Upsilon $b\bar{b}$ [12] and E_n or $E_n^{'}$. In either case, the parameters a and μ are adjusted so that E_n or $E_n^{'}$ is coinciding with $E_n^{\rm exp}$ for $n = 1$ and 2. the mass of constituent quark b is fitted as

$$m_b = 2\mu = 4.326{\rm GeV} \tag{36}$$

$$a = 0.4530{\rm GeV}^2$$

from E_n versus

$$m_b^{'} = 2\mu^{'} = 4.354{\rm GeV} \tag{37}$$

$$a^{'} = 0.3804{\rm GeV}^2$$

from $E_n^{'}$. The general trend of E_n for higher n seems better than that of $E_n^{'}$ as shown in the table.
5. Similar fitting procedure used for Charmonium $J/\psi = c\bar{c}$ by Eq.(34) leads to

$$m_c = 1.031\text{GeV} \tag{38}$$
$$a = 0.4183\text{GeV}^2$$

whereas Eq.(35) yields

$$m_c^{'} = 1.155\text{GeV} \tag{39}$$
$$a^{'} = 0.2099\text{GeV}^2$$

6. If neglecting the dependence of constant a in $V(r) = ar$ on the quark mass, we may discuss the dependence of quarkonium mass on the quark mass for the level with same quantum numbers. The Feynman-Hellmann theorem for stationary Schrö*dinger* equation reads [13]

$$\frac{\partial \epsilon}{\partial \mu} = -\frac{1}{\mu}(\epsilon - \langle V \rangle) < 0 \tag{40}$$

Now it is replaced by

$$\frac{\partial E}{\partial \mu} = -\frac{4}{E}(\epsilon - \langle V \rangle) + \frac{8\mu}{E} + \frac{E}{2\mu} \tag{41}$$

The latter two terms in RHS are positive. Combining Eq.(41) further with the virial theorem:

$$\epsilon - \langle V \rangle \equiv \langle T \rangle = \langle \frac{1}{2} r \frac{dV}{dr} \rangle \tag{42}$$

we get for $V(r) = ar$:

$$\frac{\partial E}{\partial \mu} = \frac{1}{3}\frac{E}{\mu} + \frac{32}{3}\frac{\mu}{E} \tag{43}$$

versus

$$\frac{\partial E^{'}}{\partial \mu^{'}} = \frac{16}{3} - \frac{1}{3}\frac{E^{'}}{\mu^{'}} \tag{44}$$

from $E^{'} = \epsilon + 4\mu^{'}$. Eq.(44) can easily be integrated as

$$E^{'}(\mu^{'}) = 4\mu^{'} + C^{'}\mu^{'-1/3} \tag{45}$$

whereas Eq.(43) can also be linearized by $E = \sqrt{y}$ and integrated as

$$E(\mu) = [16\mu^2 + C\mu^{2/3}]^{1/2} \tag{46}$$

As an interesting test, we use the experimental data of ground state energy for Charmonim $E_1 = 3.097$ GeV to fix the value of C in Eq.(46) or $C^{'}$ in Eq.(45) (using the value of μ or $\mu^{'}$ in the Eqs.(38) or (39) at the same time). Then the ground state of $b\bar{b}$ can be estimated as

$$E_1(b\bar{b}) = 9.420\text{GeV} \tag{47}$$

or

$$E_1^{'}(b\bar{b}) = 9.214\text{GeV} \tag{48}$$

versus

$$E_1^{\exp}(b\bar{b}) = 9.460\text{GeV} \tag{49}$$

Similarily for the $2S$ state (3.686 GeV) of Charmonium with other value of C or C', we get

$$E_2(b\bar{b}) = 9.9562\text{GeV} \tag{50}$$

$$E_2'(b\bar{b}) = 9.5922\text{GeV} \tag{51}$$

versus

$$E_2^{\exp}(b\bar{b}) = 10.023\text{GeV} \tag{52}$$

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Table 1: The S states of Upsilon $b\bar{b}$.

n	1	2	3	4	5	6
$E_n^{\rm exp}$ (GeV)	9.46037	10.023	10.355	10.580	10.865	11.019
E_n (GeV)	9.46037	10.023	10.461	10.834	11.163	11.462
$E_n^{'}$ (GeV)	9.46037	10.023	10.483	10.890	11.262	11.609
λ_n	2.338	4.088	5.521	6.787	7.944	9.023

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