Sound relativistic quantum mechanics for a strictly solitary nonzero-mass particle, and its quantum-field reverberations

Steven Kenneth Kauffmann
American Physical Society Senior Life Member

43 Bedok Road
#01-11
Country Park Condominium
Singapore 469564
Handphone: +65 9370 6583

and

Unit 802, Reflection on the Sea
120 Marine Parade
Coolangatta QLD 4225
Australia
Tel/FAX: +61 7 5536 7235
Mobile: +61 4 0567 9058

Email: SKKauffmann@gmail.com

Abstract

It is generally acknowledged that neither the Klein-Gordon equation nor the Dirac Hamiltonian can produce sound solitary-particle relativistic quantum mechanics due to the ill effects of their negative-energy solutions; instead their field-quantized wavefunctions are reinterpreted as dealing with particle and antiparticle simultaneously—despite the clear physical distinguishability of antiparticle from particle and the empirically known slight breaking of the underlying CP invariance. The natural square-root Hamiltonian of the free relativistic solitary particle is iterated to obtain the Klein-Gordon equation and linearized to obtain the Dirac Hamiltonian, steps that have calculational but not physical motivation, and which generate the above-mentioned problematic negative-energy solutions as extraneous artifacts. Since the natural square-root Hamiltonian for the free relativistic solitary particle contrariwise produces physically unexceptionable quantum mechanics, this article focuses on extending that Hamiltonian to describe a solitary particle (of either spin 0 or spin \( \frac{1}{2} \)) in relativistic interaction with an external electromagnetic field. That is achieved by use of Lorentz-covariant solitary-particle four-momentum techniques together with the assumption that well-known nonrelativistic dynamics applies in the particle’s rest frame. Lorentz-invariant solitary-particle actions, whose formal Hamiltonization is an equivalent alternative approach, are as well explicitly displayed. It is proposed that two separate solitary-particle wavefunctions, one for a particle and the other for its antiparticle, be independently quantized in lieu of “reinterpreting” negative-energy solutions—which indeed don’t even afflict proper solitary particles.
Introduction

Motivated by certain considerations of perceived calculational ease rather than by any compelling physical argument [1], Klein, Gordon and Schrödinger iterated the natural Schrödinger equation for a free relativistic solitary nonzero-mass particle,

$$i\hbar \partial |\psi\rangle / \partial t = \sqrt{m^2 c^4 + |\mathbf{p}|^2} |\psi\rangle,$$

(1)

to become,

$$-\hbar^2 \partial^2 |\psi\rangle / \partial \mathbf{p}^2 = (\sqrt{m^2 c^4 + |\mathbf{p}|^2})^2 |\psi\rangle = (m^2 c^4 + |\mathbf{p}|^2) |\psi\rangle.$$

We see that this adds to each to each stationary eigensolution \(e^{-i \sqrt{m^2 c^4 + |\mathbf{p}|^2} / \hbar t} |\mathbf{p}\rangle\) of the above relativistic free solitary-particle Schrödinger equation an extraneous negative-energy partner solution \(e^{i \sqrt{m^2 c^4 + |\mathbf{p}|^2} / \hbar t} |\mathbf{p}\rangle\). These extraneous negative “free solitary-particle” energies, \(-\sqrt{m^2 c^4 + |\mathbf{p}|^2}\), do not correspond to anything that exists in the classical dynamics of a free relativistic solitary particle, and by their negatively unbounded character threaten to spawn unstable runaway phenomena should the Klein-Gordon equation be sufficiently perturbed (the Klein paradox) [1]. Since the Klein-Gordon equation lacks a corresponding Hamiltonian, it turns out, as is easily verified, that the two solutions of the same momentum \(\mathbf{p}\) which have opposite-sign energies, i.e., \(|m^2 c^2 + |\mathbf{p}|^2| \), fail to be orthogonal to each other, which violates a key property of orthodox quantum mechanics. Without this property the probability interpretation of quantum mechanics cannot be sustained, and the Klein-Gordon equation is unsurprisingly diseased in that regard, yielding, inter alia, negative probabilities [1].

This probability disease prompted Dirac to try to replace the Klein-Gordon equation with a Hamiltonian, specifically a linearization of the natural relativistic free-particle Hamiltonian \(\sqrt{m^2 c^4 + |\mathbf{p}|^2}\) of Eq. (1) that has the postulated form \(\hat{H}_D = \alpha_0 m c^2 + \tilde{\alpha} \cdot \mathbf{p}\), where imposition on the Hermitian matrices \((\alpha_0, \alpha_1, \alpha_2, \alpha_3)\) of the anticommutation relations, \(\alpha_r \alpha_s + \alpha_s \alpha_r = 2\delta_{rs}, r, s = 0, 1, 2, 3\), ensures that [1],

$$\hat{H}_D^2 = m^2 c^4 + |\mathbf{p}|^2 = (\sqrt{m^2 c^4 + |\mathbf{p}|^2})^2.$$

Dirac’s motivation for linearizing the natural relativistic free-particle Hamiltonian \(\sqrt{m^2 c^4 + |\mathbf{p}|^2}\) was again one of perceived calculational ease rather than any compelling physical argument. The eigenenergies of Dirac’s linearized \(\hat{H}_D\) turn out to include all the extraneous negative energies which are such a vexing feature of the Klein-Gordon equation’s solutions in the context of a free solitary particle. Technically, this is a consequence of the fact that, as a matrix, \(\hat{H}_D\) is traceless because each of the four matrices \(\alpha_r, r = 0, 1, 2, 3\), is traceless, as can be demonstrated by using their anticommutation relations [1]. While the negative-energy eigenstates of \(\hat{H}_D\) are properly orthogonal to their positive-energy counterparts, the other inherent issues which the presence of these negative-energy solutions raise in the context of a free solitary particle, such as the classical limit and the Klein paradox remain unresolved [1]. In addition, straightforward calculation of the free solitary-particle velocity and consequent speed using \(\hat{H}_D\) and the Heisenberg equation of motion reveals apparent incompatibility of this Hamiltonian with special relativity (i.e., a universal free-particle speed of \(\sqrt{3}c\)) when it is interpreted as a strictly solitary-particle Hamiltonian. (On this basis one also finds that \(\hat{H}_D\) implies an egregious violation of Newton’s first law of motion for a free solitary particle, which would as well be entirely incompatible with special relativity for such a particle.)

Thus neither the Klein-Gordon equation nor the Dirac Hamiltonian are capable of sensibly describing strictly solitary-particle relativistic quantum mechanics [1]. One might have thought that this would have prompted the abandonment of those two constructs in favor of the natural relativistic free-particle Hamiltonian \(\sqrt{m^2 c^4 + |\mathbf{p}|^2}\) of Eq. (1), which is positive definite and has no problem whatsoever with sensibly describing free solitary-particle relativistic quantum mechanics. Quite to the contrary, however, the Klein-Gordon and Dirac wave functions have been duly quantized as field operators, with the Hermitian conjugates of the negative-energy parts of those quantum fields reinterpreted as antiparticle quantum fields [1]. While antiparticles are
an unquestionable feature of the physical landscape, it is as well unquestionable that antiparticles are fully distinguishable from their particle partners, a quality that would normally require any one of them to be described by a quantum field which is completely independent of the field that describes its particle partner. Furthermore, the underlying CP symmetry between particles and their antiparticle partners is empirically known to be very slightly broken (this certainly doesn't conflict with common sense in view of the notable excess of particles over antiparticles in the world around us!). Such a breaking is well-nigh impossible to achieve theoretically if the particle and its antiparticle partner both “spring” from the very same quantum field that was originally constructed to describe only the particle. However, CP symmetry breaking is theoretically achievable in myriad ways if the particle and its antiparticle partner are each described by its own independent quantum field (as one elementary example, it can be effected by introducing a tiny mass difference between those two independent fields).

In light of the above considerations, it is by no means apparent that the negative energy solutions of the Klein-Gordon and Dirac theories, which clearly preclude them from making sense in the context of strictly solitary-particle relativistic quantum mechanics, are in fact the “triumph” for the understanding of antiparticles that they are conventionally claimed to be [1]. To the contrary, it is a field-theoretic anomaly that the fully distinguishable antiparticle fails to be described by a field which is completely independent of the field that describes its particle partner, and the need for such field independence becomes pressing in view of the empirically verified breaking of particle-antiparticle CP symmetry. Now the problematic negative-energy solutions of the Klein-Gordon and Dirac theories only arose as entirely extraneous artifacts of either the physically unmotivated iteration or the likewise physically unmotivated linearization of the classical-physics-mandated natural relativistic free-particle quantum mechanics Hamiltonian $\sqrt{m^2c^4 + |\vec{p}|^2}$, which is itself entirely positive. Given the failure of those negative-energy solutions to properly fulfill their envisaged antiparticle role, which comes in addition to their extraordinarily artificial origin, it is reasonable to begin exploring possible alternatives. The one that, of course, commands our full attention is the unconditional return to the unexceptionable solitary-particle quantum mechanics implied by Eq. (1), simply because free solitary-particle classical relativistic dynamics mandates for quantum mechanics its Hamiltonian $\sqrt{m^2c^4 + |\vec{p}|^2}$! Any disrespect of the classical correspondence principle, even in very small details, is highly likely to generate wrong quantum mechanics. This extremely tight coupling of quantum to classical mechanics is implicit in the Hamiltonian path integral, which generates all quantum transition amplitudes directly from the purely classical Hamiltonian function! Now the Hamiltonian path integral hadn’t been formulated at the time that Klein, Gordon, Schrödinger and Dirac were taking liberties with Eq. (1), so the classical correspondence principle was a vastly less constraining concept in the minds of these pioneers than what the fully mature theoretical underpinning of quantum mechanics in fact implies. Even allowing for this, looking at some of the predictions of the classically-mandated relativistic quantum mechanics $\sqrt{m^2c^4 + |\vec{p}|^2}$ for the free relativistic solitary particle versus those of Dirac’s linearized version of it, i.e., $\bar{H}_D$, is starkly revealing: the former’s particle speed operator is $c|\vec{p}|/\sqrt{|\vec{p}|^2 + m^2c^2}$, which is strictly less than $c$, while the latter’s is simply $\sqrt{3}c$, a universal speed that exceeds $c$ by over 70%; the lower bound of the former’s energy is $mc^2$, while the latter’s energies are negatively unbounded; the former’s acceleration operator vanishes identically, in accord with Newton’s first law for a free particle, while the latter has a minimum acceleration magnitude of the order of the “Compton acceleration” $mc^3/\hbar$, which for the electron works out to approximately $10^{28}$ g; the nonrelativistic limit of the former is unambiguous and correct, i.e., $(\sqrt{m^2c^4 + |\vec{p}|^2} - mc^2) \rightarrow |\vec{p}|^2/(2m)$ as $c \rightarrow \infty$, a result thwarted by the negative energies of the latter; the former conserves particle orbital angular momentum, $\vec{L} = \vec{r} \times \vec{p}$, which a free particle of any spin must do, the latter does not. Dirac specifically made certain that $(\bar{H}_D)^2 = m^2c^4 + |\vec{p}|^2$, which is the same as $(\sqrt{m^2c^4 + |\vec{p}|^2})^2$, but the tolerance of quantum mechanics for any alterations of the character of its classical input can be poor in the extreme!

If we now accept the positive definite Hamiltonian $\sqrt{m^2c^4 + |\vec{p}|^2}$ as the correct description of the quantum mechanics of any free relativistic nonzero-mass solitary particle, then it obviously must similarly apply to any free solitary antiparticle, albeit, of course, with that antiparticle’s degrees of freedom. Since particle and antiparticle are fully distinguishable, their wave-function second quantization will, in the absence of any inter-
action, involve two completely independent quantum fields, whose operator evolutions are both determined by this type of first-quantized Hamiltonian. The pair-grouping of antiparticles with their particle partners is then the result of an overall field theoretic (slightly) broken CP symmetry, and is analogous to particle groupings into isospin multiplets, SU(3) octets and all the other particle groupings that are the result of broken symmetries! With regard to the “conventional” approach to antiparticles, it seems implausible theoretical physics to specifically reject the classically-mandated relativistic free solitary-particle quantum mechanics Hamiltonian \( \sqrt{m^2c^4 + |p|^2} \), that has positive definite energy, simply in order to make use of its physically unmotivated and apparently defective Klein-Gordon and Dirac offshoots for the express purpose of inventing from whole cloth a scheme of “partial-quantum-field negative-energy reinterpretation” that only applies to the pair-grouping of antiparticles with their particle partners amongst all the similar particle-grouping schemes that contrariwise are due to broken symmetries, and that appears to be not capable of coexisting with the circumstantially expected and empirically verified breaking of the underlying CP symmetry.

Whereas the Hamiltonian \( \sqrt{m^2c^4 + |p|^2} \) provides a physically sensible description of the relativistic quantum mechanics of a free nonzero-mass solitary particle (and also of such a free solitary antiparticle), the focus of this article lies beyond the merely free relativistic solitary particle: it is on working out Hamiltonians which describe physically sensible relativistic quantum mechanics for such a solitary particle (of either spin 0 or spin \( \frac{1}{2} \)) in interaction with an external electromagnetic field. First, however, we need to learn how to get past the technical stumbling block that neither Hamiltonians nor the familiar usual form of the Schrödinger equation are themselves manifestly Lorentz covariant.

The four-momentum method in relativistic solitary-particle mechanics

When a solitary particle of nonzero mass \( m \) interacts with external fields, its relativistic Hamiltonian is of the general form \( H(x, P, t; m) \), where \( x \) is the vector of the particle’s three position coordinates and \( P \) is its total dynamical three-momentum, i.e., the sum of its kinetic three-momentum \( p \) with any three-momentum contributions that arise from its interaction with the external fields. The reason for the occurrence of the particle’s total dynamical three-momentum \( P \) in its Hamiltonian is that the total three-momentum of any physical system generates the translations of that system’s center-of-mass coordinates \( x_{CM} \). For the solitary particle, obviously \( x_{CM} = x \), and the fact that \( P \) generates the translations of \( x \) implies that the three components of \( P \) are canonically conjugate to the three corresponding components of \( x \). Therefore it is the the solitary particle’s total dynamical three-momentum \( P \) that properly belongs in its Hamiltonian \( H(x, P, t; m) \). Furthermore, the total dynamical four-momentum of the solitary particle is obviously \( P^\mu \equiv (H(x, P, t; m)/c, P) \). Special relativity of course imposes on \( P^\mu \) the requirement that it transform between inertial frames as a Lorentz-covariant four-vector.

The inherently four-momentum character of solitary-particle relativistic dynamics naturally carries over to its quantum mechanics. The quantum expression of the canonically conjugate character of \( x \) to \( P \) is, of course, the familiar commutation relation, \( [[\hat{x}]]^\mu, (\hat{P}^\nu)] = i\hbar\gamma^\nu \mathbf{I} \), which, in configuration representation, implies the familiar relation, \( \langle x|\hat{P}^\mu|\psi(t)\rangle = -i\hbar\nabla_x\langle x|\psi(t)\rangle \). This, when combined with the relativistic solitary-particle Schrödinger equation, \( i\hbar\partial\langle x|\psi(t)\rangle/\partial t = \langle x|H|\psi(t)\rangle \), produces the formal quantum-mechanical equality of two four-vectors,

\[
\langle x|\hat{P}^\mu|\psi(t)\rangle = i\hbar\partial\langle x|\psi(t)\rangle/\partial x^\mu = \langle x|\hat{P}^\mu|\psi(t)\rangle,
\]

where the covariant components of \( x^\mu = (ct, -\mathbf{x}) \). It is interesting to note that iteration of this four-momentum Schrödinger equation, followed by index contraction, produces the Lorentz-invariant generalization of the Klein-Gordon equation, \( \partial^\mu\partial_\mu(x|\psi(t)\rangle = -\langle x|\hat{P}^\mu\hat{P}_\mu|\psi(t)\rangle/\hbar^2 \). Of course this Lorentz scalar equation can not be expected to imply the above Lorentz four-vector Schrödinger equation, and the iteration which is part of its derivation can be expected to burden it with extraneous, unphysical solutions (at least in the strictly solitary-particle regime), such as the negative-energy ones which have been previously noted above in the free-particle situation that \( \hat{P}^\mu = \hat{p}^\mu = (\sqrt{m^2c^4 + |p|^2}, \mathbf{p}) \).
The relativistic free particle is, of course, a special case of the relativistic solitary particle, whose total dynamical three-momentum $\mathbf{P}$ consists of only its kinetic three-momentum $\mathbf{p}$, which has a value that depends on the choice of inertial frame from which it is viewed in accord with the rules of special relativity for a free particle of nonzero mass $m$. Thus when viewed from the free particle’s rest frame, $\mathbf{p} = 0$, whereas when viewed from an inertial frame in which the free particle has velocity $\mathbf{v}$, the free particle’s kinetic momentum $\mathbf{p}$ is equal to $mv\gamma$, where the Lorentz time dilation factor $\gamma \equiv 1/\sqrt{1 - \mathbf{v}^2}$. We therefore calculate that to Lorentz boost the free particle from rest to kinetic three-momentum $\mathbf{p}$ involves the Lorentz time dilation factor $\gamma(\mathbf{p}) = \sqrt{1 + |\mathbf{p}/(mc)|^2}$ and the Lorentz boost velocity $\mathbf{v}(\mathbf{p}) = \mathbf{c}p/\sqrt{m^2c^2 + |\mathbf{p}|^2}$. We recall from the preceding paragraph that the free particle’s dynamical three-momentum $\mathbf{P}$ must Lorentz transform between these two inertial frames as a covariant four-vector. In the free particle’s rest frame, $\mathbf{p} = (H_{\text{free}}(\mathbf{x}, \mathbf{p}, t; m)/c, \mathbf{p})$ involves the Lorentz boost matrix, $\Lambda_0^\mu(\mathbf{v}(\mathbf{p})) = (\gamma(\mathbf{p}), \gamma(\mathbf{p})\mathbf{v}(\mathbf{p})/c) = (\sqrt{1 + |\mathbf{p}/(mc)|^2}/c, \mathbf{p}/(mc))$. This produces the boosted free-particle four-momentum, $(H_{\text{free}}(\mathbf{x}, 0, t; m)/c, H_{\text{free}}(\mathbf{x}, 0, t; m))$, which is, of course, required by the above-stated imposition of Lorentz covariance to be equal to, $\mathbf{p}^\mu \equiv (H_{\text{free}}(\mathbf{x}, \mathbf{p}, t; m)/c, \mathbf{p})$. Therefore Lorentz covariance of the free-particle four-momentum implies that $H_{\text{free}}(\mathbf{x}, 0, t; m) = mc^2$, and, furthermore, that, $H_{\text{free}}(\mathbf{x}, \mathbf{p}, t; m) = \sqrt{m^2c^4 + |\mathbf{p}|^2}$. Thus we see that the imposition of special relativity completely determines the Hamiltonian $H_{\text{free}}(\mathbf{x}, \mathbf{p}, t; m)$ of any free particle of nonzero mass $m$ to be $\sqrt{m^2c^4 + |\mathbf{p}|^2}$. This uniqueness of the relativistic $H_{\text{free}}$ in classical relativistic dynamics obviously also enforces Eq. (1) as the correct quantum mechanical description of a free relativistic nonzero-mass solitary particle.

For completeness we point out that $H_{\text{free}}$ can also be worked out from the extraordinarily simple-looking Lorentz-invariant action for the solitary free particle,

$$\int d\tau (-mc^2),$$

where $d\tau$ is the solitary particle’s differential proper time interval, which is defined via the particle’s space-time contravariant four-vector location $x^\mu = (\tau, \mathbf{x})$ and,

$$(d\tau)^2 \equiv dx^\mu dx_\mu/c^2 = (dt)^2 - |d\mathbf{x}/c|^2.$$

Therefore the relativistic Lagrangian $L$ for the free particle follows from its above Lorentz-invariant action as, $L = (-mc^2)d\tau/dt = (-mc^2)\sqrt{1 - |\mathbf{x}/c|^2} = (-mc^2)/\gamma$, where $\gamma \equiv 1/\sqrt{1 - |\mathbf{x}/c|^2}$ is the usual Lorentz time-dilation factor. With the Lagrangian $L$ in hand, we can work out the free-particle canonical momentum in the usual way,

$$\mathbf{p} = \nabla_{\mathbf{x}}L = mc\gamma.$$

Continuing along these lines in classical dynamics textbook fashion permits us to eventually calculate the free-particle Hamiltonian $H_{\text{free}}$, but the process is astonishingly long-winded, in contrast with the stark simplicity of the above Lorentz-invariant action and its Lorentz-invariant “time-dilated Lagrangian”, $-mc^2$. 

5
Development of relativistic Hamiltonians for interacting solitary particles

Knowing that any solitary free particle of nonzero mass $m$ is described by the familiar relativistic square-root Hamiltonian, $H_{\text{free}} = \sqrt{m^2c^4 + |\mathbf{p}|^2}$ and four-momentum $\mathbf{p}^\mu = (\mathbf{H}_{\text{free}}, \mathbf{p})$, we now turn to the development of relativistic Hamiltonians for such a solitary particle in interaction with external fields. For an external electromagnetic field there do exist nonrelativistic Hamiltonians for the spinless and spin $\frac{1}{2}$ charged particle which are considered trustworthy, and it is physically clear that for a solitary particle the correct nonrelativistic Hamiltonian ought to actually determine its fully relativistic counterpart! That is because the correct nonrelativistic Hamiltonian ought to be absolutely precise in the instantaneous rest frame of the particle. This line of physical reasoning seems more a route toward relativistic upgrading of the dynamics itself rather than the Hamiltonian directly, albeit the latter can presumably always be extracted from the former.

A direct relativistic upgrade of any term of a nonrelativistic Hamiltonian would involve crafting a properly Lorentz-covariant four-momentum whose nought component times $c$ reduces to that particular term of the nonrelativistic Hamiltonian in the particle’s rest frame. If this is done for all the terms which make up the nonrelativistic Hamiltonian, then all those four-momenta are to be added together. As was discussed in the previous section, the resulting total three-momentum will be canonically conjugate to the three components of the particle’s position vector. The resulting total energy therefore becomes the interacting particle’s Hamiltonian if its dependence on the particle’s kinetic three-momentum can be reexpressed as dependence on its total three-momentum, i.e., we need to solve for the kinetic three-momentum as a function of the total three-momentum and then substitute this function into the total energy, which thereupon becomes the particle’s relativistic Hamiltonian. It cannot be guaranteed, of course, that the particle’s kinetic momentum can be obtained as a function of its total momentum in closed form. If this function cannot be obtained in closed form, successive iteration approximations to it are sometimes adequate.

Before turning to our first example of this approach, we must note a slight but universal exception to the rule that the nought component times $c$ of each of our Lorentz-covariant four-momenta reduces in the particle’s rest frame to a corresponding term of the nonrelativistic Hamiltonian in the particle’s rest frame. The resulting total energy therefore becomes the interacting particle’s Hamiltonian if its dependence on the particle’s kinetic three-momentum can be reexpressed as dependence on its total three-momentum, i.e., we need to solve for the kinetic three-momentum as a function of the total three-momentum and then substitute this function into the total energy, which thereupon becomes the particle’s relativistic Hamiltonian. It cannot be guaranteed, of course, that the particle’s kinetic momentum can be obtained as a function of its total momentum in closed form. If this function cannot be obtained in closed form, successive iteration approximations to it are sometimes adequate.

Relativistic Hamiltonian for the spinless charged solitary particle

A completely nonrelativistic spinless charged particle which interacts with an external electromagnetic field is described by the Hamiltonian,

$$H_{\text{EM};0}^{\text{(NR)}} = |\mathbf{p}|^2/(2m) + eA^0(\mathbf{x}, t). \tag{2}$$

Now in order to take account of the interaction of a nonrelativistic spinless charged particle with an external magnetic field, the Hamiltonian of Eq. (2) is often upgraded to a partially relativistic form which involves the electromagnetic vector potential $\mathbf{A}$ occurring in conjunction with the speed of light $c$ in a term of the form $e\mathbf{A}(\mathbf{x}, t)/c$. Such terms of course vanish in the limit that $c \to \infty$, which is why we have left them out of the completely nonrelativistic Hamiltonian of Eq. (2): we shall see that they are a natural consequence of the full relativistic upgrade of the Hamiltonian of Eq. (2) that we are about to undertake.

As we have discussed at the end of the previous section, the kinetic energy term $|\mathbf{p}|^2/(2m)$ of the nonrelativistic Hamiltonian $H_{\text{EM};0}^{\text{(NR)}}$ of Eq. (2) corresponds to the free-particle four-momentum, $p^\mu = (\sqrt{m^2c^2 + |\mathbf{p}|^2}, \mathbf{p})$. The potential energy term $eA^0(\mathbf{x}, t)$ of this nonrelativistic Hamiltonian involves the nought component $A^0$ of
the full electromagnetic four-potential \( A^\mu \). Therefore the Lorentz covariant four-momentum which corresponds to the potential energy term \( eA^0(x, t) \) of this nonrelativistic Hamiltonian is, \( eA^\mu(x, t)/c \). Thus the total four-momentum \( P^\mu \) of our relativistically upgraded system is,

$$ P^\mu = p^\mu + eA^\mu(x, t)/c. $$

From this we read off the total three-momentum of our relativistic system,

$$ \mathbf{P} = \mathbf{p} + e \mathbf{A}(x, t)/c, $$

and its total energy,

$$ E(x, \mathbf{p}, t) = \sqrt{m^2c^4 + |\mathbf{p}|^2 + eA^0(x, t)}. $$

We now recall from the previous section that in order to obtain the relativistic Hamiltonian \( H(x, \mathbf{P}, t) \) we must solve for the kinetic three-momentum \( \mathbf{p} \) as a function of the total three-momentum \( \mathbf{P} \), i.e., we must solve for \( \mathbf{p}(\mathbf{P}) \), which when put into the total energy \( E(x, \mathbf{p}, t) \), yields the relativistic Hamiltonian \( H(x, \mathbf{P}, t) \) as,

$$ H(x, \mathbf{P}, t) = E(x, \mathbf{p}(\mathbf{P}), t). $$

Fortunately, in this instance we are easily able to obtain \( \mathbf{p}(\mathbf{P}) \) in closed form, namely, \( \mathbf{p}(\mathbf{P}) = \mathbf{P} - e \mathbf{A}(x, t)/c \). Therefore we obtain the full relativistic upgrade of the Hamiltonian of the spinless charged particle in interaction with an external electromagnetic four-potential,

$$ H_{\text{EM};0}^{(\text{REL})} = \sqrt{m^2c^4 + |\mathbf{P} - e \mathbf{A}(x, t)|^2 + eA^0(x, t)}. \quad (3) $$

It is clear that as \( c \to \infty, (H_{\text{EM};0}^{(\text{REL})} - mc^2) \to H_{\text{EM};0}^{(\text{NR})} \). We also note that since the argument of the square root in Eq. (3) is a joint function of \( \mathbf{P} \) and \( x \), the operator ordering ambiguity which is a consequence of Dirac’s original widely accepted canonical commutation rules has the potential to present a considerable annoyance for the quantization of \( H_{\text{EM};0}^{(\text{REL})} \). Fortunately, however, both the Hamiltonian path integral \( \mathbb{Z} \) and a self-consistent slight strengthening of Dirac’s original canonical commutation rules \( \mathbb{Z} \) have been shown to yield exactly the same completely unambiguous Born-Jordan quantization of all classical dynamical variables; this aspect of quantization would appear to be of considerably greater practical relevance to relativistic quantum mechanics than to its nonrelativistic counterpart. It may be of interest to the reader that Dirac’s well-known but inadequate phase-space-vector Cartesian-component canonical commutation rules are to be replaced by the slightly stronger, but still self-consistent, canonical commutation rule \( \mathbb{Z} \),

$$ [f_1(\bar{x}) + g_1(\bar{P}), f_2(\bar{x}) + g_2(\bar{P})] = i\hbar \left( \nabla_\mathbf{x} f_1(\bar{x}) \cdot \nabla_\mathbf{P} g_2(\bar{P}) + \nabla_\mathbf{x} g_1(\bar{P}) \cdot \nabla_\mathbf{P} f_2(\bar{x}) \right), $$

where both the hat accent and the overbrace are used to indicate the quantization of a classical dynamical variable.

It is furthermore apparent that the classical Hamiltonian equations of motion which the \( H_{\text{EM};0}^{(\text{REL})} \) of Eq. (3) implies are simply those of the very well-known fully relativistic Lorentz force \( \mathbb{Z} \). For completeness we also mention that the corresponding Lorentz-invariant action is the quite well-known,

$$ \int d\tau (-mc^2 - (e/c)A_\mu(x^\nu)dx^\mu/d\tau), $$

and from it \( H_{\text{EM};0}^{(\text{REL})} \) can as well be calculated by a somewhat tedious standard sequence of classical dynamics steps. The pattern that emerges here for the solitary spinless particle in fully relativistic interaction with an external electromagnetic field is a precise relationship to well-known classical relativistic dynamics which the Klein-Gordon equation cannot even begin to achieve. This precise classical relativistic correspondence lends impressive support to the quantization of \( H_{\text{EM};0}^{(\text{REL})} \) being the correct quantum mechanics description of a relativistic spinless nonzero-mass charged solitary particle in interaction with an external electromagnetic field, and validates the methodology whereby the relativistic Eq. (3) was derived from the nonrelativistic Eq. (2).
Relativistic Hamiltonian for the spin $\frac{1}{2}$ charged particle

We now turn to the relativistic upgrade of the nonrelativistic Pauli Hamiltonian for the interaction of a charged particle of spin $\frac{1}{2}$ and specified magnetic moment $g$-factor with an external electromagnetic four-potential $(A^0, \mathbf{A})$,

$$H_{\text{Pauli}} = H_{\text{EM;}\frac{1}{2}}^{(NR)} = |\mathbf{p} - e\mathbf{A}(x,t)/c|^2/(2m) + eA^0(x,t) + (ge/(mc))(\hbar/2)\tilde{\sigma} \cdot (\nabla_x \times \mathbf{A}(x,t)).$$

There are some points to bear in mind about $H_{\text{EM;}\frac{1}{2}}^{(NR)}$. First it is already partially relativistic. Note that if we take the limit $c \to \infty$, $H_{\text{EM;}\frac{1}{2}}^{(NR)} \to H_{\text{EM;}0}^{(NR)}$, i.e., we lose the electromagnetic field’s interaction with spin $\frac{1}{2}$ just as surely in the the fully nonrelativistic limit as we lose it in the the $\hbar \to 0$ classical limit. It is apparent that $H_{\text{EM;}\frac{1}{2}}^{(NR)}$ must retain relativistic effects through order $O(1/c)$ in order to be able to describe the magnetic moment coupling of spin $\frac{1}{2}$. Second, $H_{\text{EM;}\frac{1}{2}}^{(NR)}$ is a Hermitian two-by-two matrix. Therefore the relativistic four-momenta we intend to develop must be such matrices as well. That should not be a problem so long as we do not generate four-momentum components that fail to mutually commute. Therefore it would be prophylactic to quarantine the one intrinsically two-by-two matrix term of $H_{\text{EM;}\frac{1}{2}}^{(NR)}$ i.e., the spin-$\frac{1}{2}$/magnetic-field interaction, $(ge/(mc))(\hbar/2)\tilde{\sigma} \cdot (\nabla_x \times \mathbf{A}(x,t))$, within a Lorentz invariant. This, however, raises the issue that we wish such nonrelativistic Hamiltonian terms to correspond to $c$ times the nought component of a four-momentum in the particle’s rest frame, not to a Lorentz invariant. But that turns out to be quite easily arranged once the Lorentz invariant is in hand: we simply divide that Lorentz-invariant spin interaction energy by $mc^2$, and then multiply the resulting dimensionless Lorentz-invariant object by the $\text{free-particle}$ four-momentum $p^\mu = (\sqrt{m^2c^2 + |\mathbf{p}|^2}, \mathbf{p})$, where $\mathbf{p}$ is, of course, the particle’s kinetic three-momentum.

From our work in the previous section with $H_{\text{EM;}0}^{(REL)}$, we recognize that the “partially relativistic” kinetic energy term of $H_{\text{EM;}\frac{1}{2}}^{(NR)}$, namely, $|\mathbf{p} - e\mathbf{A}(x,t)/c|^2/(2m)$, still simply corresponds to the usual free-particle four-momentum, namely $p^\mu = (\sqrt{m^2c^2 + |\mathbf{p}|^2}, \mathbf{p})$. We of course immediately as well recognize that the term $eA^0(x,t)$ of $H_{\text{EM;}\frac{1}{2}}^{(NR)}$ corresponds to the four-momentum, $eA^0(x,t)/c$.

Now comes the difficult part: we are to quarantine the one intrinsically two-by-two matrix term of $H_{\text{EM;}\frac{1}{2}}^{(NR)}$, namely, $(ge/(mc))(\hbar/2)\tilde{\sigma} \cdot (\nabla_x \times \mathbf{A}(x,t))$, within a Lorentz invariant. To move toward that goal, we note that the Lorentz covariant form of the electromagnetic field is the second-rank antisymmetric tensor $F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$. Now we can write a magnetic-field axial vector component from $H_{\text{EM;}\frac{1}{2}}^{(NR)}$, namely, $(\nabla_x \times \mathbf{A})^i$, as,

$$(\nabla_x \times \mathbf{A})^i = \epsilon^{ijk}\partial^j A^k = \frac{1}{2}\epsilon^{ijk}(\partial^j A^k - \partial^k A^j) = \frac{1}{2}\epsilon^{ijk}F^{jk}.$$  

Therefore we obtain that,

$$(\hbar/2)\tilde{\sigma} \cdot (\nabla_x \times \mathbf{A}) = \frac{1}{2}(\hbar/2)\sigma^i\epsilon^{ijk}F^{jk} = \frac{1}{2}(\hbar/2)\epsilon^{ijk}\sigma^i F^{jk}.$$  

We now define, for the particle in its rest frame, the second-rank antisymmetric spin tensor, $S^{jk} \overset{\text{def}}{=} (\hbar/2)\epsilon^{jki}\sigma^i$. Then $(\hbar/2)\tilde{\sigma} \cdot (\nabla_x \times \mathbf{A}) = \frac{1}{2}S^{jk}F^{jk}$. To reach our final goal, we must define a Lorentz covariant $s^{\mu\nu}$ such that $s^{\mu\nu}F_{\mu\nu}$ reduces to $S^{jk}F_{jk}$ in the particle’s rest frame. We need only specify $s^{\mu\nu}$ in a single inertial frame for it to be uniquely defined: it is then obtained in any inertial frame via the appropriate Lorentz transformation. So let us simply specify $s^{\mu\nu}$ in the particle’s rest frame as follows: $s^{00} = 0$, $s^{0i} = s^{i0} = 0$, and $s^{ij} = S^{ij} = (\hbar/2)\epsilon^{jik}\sigma^k$, $i,j = 1,2,3$. With that definition, we do indeed have that $s^{\mu\nu}F_{\mu\nu}$ reduces to $S^{jk}F_{jk}$ in the particle’s rest frame. To obtain $s^{\mu\nu}$ in the frame where the particle has kinetic three-momentum $\mathbf{p}$, we must apply the appropriate Lorentz boost to its two indices,

$$s^{\mu\nu}(\mathbf{p}) = \Lambda^{\mu}_\nu(\mathbf{v}(\mathbf{p}))\Lambda^{\nu}_\sigma(\mathbf{v}(\mathbf{p}))(\hbar/2)\epsilon^{ijk}\sigma^k,$$  

(5)
where, of course, the Lorentz boost velocity \( \mathbf{v}(\mathbf{p}) = c\mathbf{p}/\sqrt{m^2c^4 + |\mathbf{p}|^2} \) and the Lorentz time dilation factor 
\( \gamma(\mathbf{p}) = \sqrt{1 + |\mathbf{p}|/(mc)^2} \). We note that the antisymmetry of \( e^{\mu \nu} \) in its two indices \( i \) and \( j \) implies that \( s^{\mu \nu}(\mathbf{p}) \) is an antisymmetric tensor in its two indices \( \mu \) and \( \nu \).

Thus the two-by-two matrix spin \( \frac{1}{2} \) interaction term of \( H_{\text{EM;NR}}^{(1)}(x, \mathbf{p}, t) \), namely \((ge/(mc))(\nabla_x \times \mathbf{A}(x, t))\), is now safely quarantined as the Lorentz invariant \((g/2)(e/(mc))s^{\mu \nu}(\mathbf{p})F_{\mu \nu}(x, t)\). We proceed to write down the corresponding four-momentum for this term by following the instructions that were given above, namely to divide this Lorentz invariant by \( mc^2 \) and then multiply the result into the free-particle four-momentum \( p^\mu \). With that, we are now in a position to write down the total four-momentum,
\[
P^\mu = p^\mu(1 + (g/2)(e/(m^2c^3))s^{\alpha \beta}(\mathbf{p})F_{\alpha \beta}(x, t)) + eA^\mu(x, t)/c,
\]
from which we obtain the total energy,
\[
E(x, \mathbf{p}, t) = \sqrt{m^2c^4 + |\mathbf{p}|^2}(1 + (g/2)(e/(m^2c^3))s^{\mu \nu}(\mathbf{p})F_{\mu \nu}(x, t)) + eA^0(x, t),
\]
and the total three-momentum,
\[
\mathbf{P} = \mathbf{p}(1 + (g/2)(e/(m^2c^3))s^{\mu \nu}(\mathbf{p})F_{\mu \nu}(x, t)) + e\mathbf{A}(x, t)/c.
\]

It is obvious from Eq. (7) that we cannot solve for \( \mathbf{p}(\mathbf{P}) \) in closed form, but we can write \( \mathbf{p}(\mathbf{P}) \) in "iteration-ready" form as,
\[
\mathbf{p}(\mathbf{P}) = (\mathbf{P} - e\mathbf{A}(x, t)/c)(1 + (g/2)(e/(m^2c^3))s^{\mu \nu}(\mathbf{p}(\mathbf{P}))F_{\mu \nu}(x, t))^{-1},
\]
and, of course, from \( E(x, \mathbf{p}(\mathbf{P}), t) \), we also obtain the schematic form of the relativistic Hamiltonian,
\[
H_{\text{EM;R}}^{(\text{REL})}(x, \mathbf{P}, t) = \sqrt{m^2c^4 + |\mathbf{p}(\mathbf{P})|^2}(1 + (g/2)(e/(m^2c^3))s^{\mu \nu}(\mathbf{p}(\mathbf{P}))F_{\mu \nu}(x, t)) + eA^0(x, t).
\]

If we take the limit \( g \rightarrow 0 \) in Eqs. (8) and (9), then \( H_{\text{EM;R}}^{(\text{REL})}(x, \mathbf{P}, t) \rightarrow H_{\text{EM;NR}}^{(\text{REL})}(x, \mathbf{P}, t) \), as is easily checked from Eq. (3). Of course it is nothing more than the most basic common sense that fully relativistic spin \( \frac{1}{2} \) theory simply reduces to fully relativistic spinless theory when the spin coupling of the single particle to the external field is switched off, but analogous cross checking between the Dirac and Klein-Gordon theories is never even discussed! It may also be checked that \((H_{\text{EM;R}}^{(\text{REL})} - mc^2)\) agrees with the “partially relativistic” Pauli \( H_{\text{EM;NR}}^{(\text{REL})} \) through terms of order \( O(1/c) \) in the limit \( c \rightarrow \infty \).

It is unfortunate that Eq. (8) for \( \mathbf{p}(\mathbf{P}) \) is not amenable to closed-form solution, but if we assume that the spin coupling term, \((g/2)(e/(m^2c^3))s^{\mu \nu}(\mathbf{p}(\mathbf{P}))F_{\mu \nu}(x, t)\), which is a dimensionless Hermitian two-by-two matrix, effectively has the magnitudes of both of its eigenvalues much smaller than unity (which should be a very safe assumption for atomic physics), then we can approximate \( \mathbf{p}(\mathbf{P}) \) via successive iterations of Eq. (8), which produces the approximation \((\mathbf{P} - e\mathbf{A}(x, t)/c) \) for \( \mathbf{p}(\mathbf{P}) \) through zeroth order in the spin coupling and,
\[
\mathbf{p}(\mathbf{P}) \approx (\mathbf{P} - e\mathbf{A}(x, t)/c)(1 + (g/2)(e/(m^2c^3))s^{\mu \nu}(\mathbf{P} - e\mathbf{A}(x, t)/c)F_{\mu \nu}(x, t))^{-1},
\]
through first order in the spin coupling. We wish to interject at this point that since \( s^{\mu \nu}(\mathbf{p}(\mathbf{P})) \) is an antisymmetric tensor, the tensor contraction \( s^{\mu \nu}(\mathbf{p}(\mathbf{P}))F_{\mu \nu}(x, t) \) is equal to \( 2s^{\mu \nu}(\mathbf{p}(\mathbf{P}))\partial_{\mu}A_{\nu}(x, t) \), which is often a more transparent form. Now if we simply use the approximation \((\mathbf{P} - e\mathbf{A}(x, t)/c) \) through zeroth order in the spin coupling for \( \mathbf{p}(\mathbf{P}) \), we obtain the following approximation to \( H_{\text{EM;R}}^{(\text{REL})}(x, \mathbf{P}, t) \),
\[
H_{\text{EM;R}}^{(\text{REL})}(x, \mathbf{P}, t) \approx \sqrt{m^2c^4 + |\mathbf{P} - e\mathbf{A}(x, t)|^2}(1 + (ge/(m^2c^3))s^{\mu \nu}(\mathbf{P} - e\mathbf{A}(x, t)/c)\partial_{\mu}A_{\nu}(x, t)) + eA^0(x, t).
\]
For completeness we also point out the corresponding Lorentz-invariant action might plausibly be,

\[ \int d\tau \left( -mc^2(1 + (g/2)(e/(m^2c^3))(dx^\alpha/d\tau)F_{\mu\nu}(x^\beta)) - (e/c)A_\mu(x^\beta)dx^\mu/d\tau \right), \]

where \( s^{\mu\nu}(c, 0) \) in the particle’s rest frame is specified as follows: \( s^{00}(c, 0) = 0, \ s^{0i}(c, 0) = s^{i0}(c, 0) = 0, \) and \( s^{ij}(c, 0) = (\hbar/2)e^{ijk}\sigma^k, \ i, j = 1, 2, 3. \) If the above guess for the Lorentz-invariant action is correct, then in principle \( H^{(\text{EM})}_{\text{REL}; \frac{1}{2}} \) can be tediously worked out from it, but we assuredly recommend against trying to proceed by that route. It is very clear indeed that the Lorentz-covariant four-momentum approach keeps one in vastly better contact with crucial physics than does trying to guess the invariant action. Furthermore, even a correct guess of that action is separated by what is always a very considerable and tedious calculational distance from the desired Hamiltonian. The four-momentum method seems in all respects the best approach to upgrading nonrelativistic solitary-particle Hamiltonians to relativistic ones.

With \( A(x, t) = 0 \) and \( A^0(x, t) = -e/|x|, \) relativistic and spin corrections to the nonrelativistic hydrogen atom energy spectrum can be investigated by regarding \( (\hat{H}^{(\text{REL})}_{\text{EM}; \frac{1}{2}} - mc^2 - \hat{H}^{(\text{NR})}_{\text{EM}; 0}) \) as a perturbation of the familiar spinless nonrelativistic Hamiltonian \( \hat{H}^{(\text{NR})}_{\text{EM}; 0} \) whose exact bound state solutions are well-known, and to which \( (\hat{H}^{(\text{REL})}_{\text{EM}; \frac{1}{2}} - mc^2) \) clearly reduces as \( c \to \infty. \) The effect of spin on the hydrogen energy spectrum arises from the fact that \( s^{ij}(p(P)) \) doesn’t vanish if \( p(P) \) is nonzero, i.e., a moving spin \( \frac{1}{2} \) particle has spin coupling to an external electric field. Another way to see this is to realize that a purely electric field in an inertial frame in which the particle is moving gives rise to a magnetic field in the particle’s rest frame, which thus activates the nonrelativistic Pauli spin coupling in that rest frame.

**Conclusion**

The discussion just above is a pertinent reminder that our fully relativistic single particle Hamiltonians \( H^{(\text{REL})}_{\text{EM}; 0} \) and \( H^{(\text{REL})}_{\text{EM}; \frac{1}{2}} \) have been completely founded on the premise that well-known nonrelativistic single-particle electromagnetic interactions are exact in the particle’s rest frame. Their only additional input was the requirement of strict Lorentz covariance. It is thus no accident that, for example, the classical Hamiltonian equations of motion which are implied by \( H^{(\text{REL})}_{\text{EM}; 0} \) are precisely those of the fully relativistic Lorentz force law for a single charged particle. The fully relativistic single-particle electromagnetic Hamiltonians \( H^{(\text{REL})}_{\text{EM}; 0} \) and \( H^{(\text{REL})}_{\text{EM}; \frac{1}{2}} \) thus represent the epitome of theoretical physics conservatism in the realm of an electromagnetically interacting relativistic solitary particle.

**References**

[1] J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* (McGraw-Hill, New York, 1964).

[2] E. H. Kerner and W. G. Sutcliffe, J. Math. Phys. **11**, 391 (1970).

[3] S. K. Kauffmann, [arXiv:0908.3755](https://arxiv.org/abs/0908.3755) [quant-ph] (2009).

[4] L. D. Landau and E. M. Lifshitz, *The Classical Theory of Fields* (Butterworth-Heinemann, Oxford, 1975).