Comments on Bound States in QFT

Paul Hoyer 7 February 2025

A. Motivations

The Schrödinger equation was central in the establishment of Quantum Mechanics 100 years ago. The Hydrogen atom remains a prime illustration in introductory courses on QM. Today we know that the Standard Model, and especially its QED and QCD sectors, provide the basic theory for atomic and hadronic states. Nature is built from bound states, but they are omitted in textbooks on Quantum Field Theory. QFT has become a theory of scattering [1].

Various QFT methods for atoms emerged gradually [2]. An expansion based on non-relativistic effective field theory (NRQED) gives impressive agreement with the Positronium spectrum. Atoms in motion and strongly bound hadrons are incompatible with a non-relativistic expansion. This motivates to consider the basics of QFT bound states.

Poincaré symmetry is realized dynamically (through interactions) for states defined at equal time (or equal light-front time $x^+ = t+z$). The quantization surface changes under boosts (or rotations at equal x^+). For example, the Lorentz contraction of classical relativity is non-trivial for atomic states (and rarely discussed). The Dirac equation for an electron in an external potential gives valuable insights, but the potential breaks space translation invariance.

QFT bound states are often discussed in terms of Feynman diagrams, following Bethe and Salpeter [3]. The free *in* and *out* states are appropriate boundary conditions for scattering, but not for bound states. An infinite sum of Feynman diagrams is required to generate a bound state pole, and the ordering of the sum is not unique [4].

The Schrödinger equation describes electron states in a classical potential. The same equation also describes heavy quarkonia with the potential $V(r) = c\,r - C_F\,\alpha_s/r$ [5], later found to agree with lattic QCD [6]. The scale $\Lambda_{QCD} \sim \sqrt{c}$ does not appear in the QCD Lagrangian.

QFT bound states can be addressed using canonical quantization in temporal ($A^0 = 0$) gauge [7–9]. Data motivates to start from "valence" states, *e.g.*, $|e^+e^-\rangle$, $|q\bar{q}\rangle$ or $|qqq\rangle$, that are eigenstates of momentum P and energy H. The Fock state constituents have instantaneous interactions in temporal gauge. Higher Fock states created by the Hamiltonian are added perturbatively in the coupling. Being based on QFT methods, and with the Λ_{QCD} scale introduced through a boundary condition, the approach preserves the Poincaré symmetry of the action.

B. Instantaneous interactions

QFT interactions are generally mediated by particle exchange. Gauge theories also have an instantaneous interaction, *cf.* the photon propagator in Coulomb gauge: The photon seemingly propagates with infinite velocity. In non-gauge theories the exchange of a light particle can mimic an instantaneous potential for heavy, non-relativistic constituents. But in gauge theories there are instantaneous interactions even between relativistic constituents.

Gauge theory actions have no $\partial_t A^0$ nor $\boldsymbol{\nabla}\cdot\boldsymbol{A}$ terms. This means that the A^0 and longitudinal $\boldsymbol{A}_L$ fields do not propagate in spacetime. In covariant (Feynman) gauge the gauge fixing term $\propto (\partial_\mu A^\mu)^2$ adds the missing derivatives, allowing all components of A^μ to propagate. This makes each Feynman diagram explicitly Poincaré invariant.

For bound states defined at an instant of time only space translations and rotations are kinetic (free of interactions). Both the Coulomb gauge $\boldsymbol{\nabla}\cdot\boldsymbol{A}(t,\boldsymbol{x}) = 0$ and temporal gauge $A^0(t,\boldsymbol{x}) = 0$ conditions preserve these symmetries. Coulomb gauge is the common choice for bound states, even though canonical quantization is problematic: the conjugate field of A^0 vanishes, $\delta S/\delta(\partial_t A^0) = 0$. In temporal gauge both A^0 and its conjugate field vanish, and the canonical quantization of the space components $\boldsymbol{A}(t,\boldsymbol{x})$ is straightforward [10].

Fixing the gauge at all space points $\boldsymbol{x}$ at an instant of time t enables instantaneous interactions without particle exchange. This is helpful for bound states because particle exchange implies higher Fock states. *E.g.,* in the absence of an instantaneous interaction the binding of a $q\bar{q}$ state requires a $q\bar{q}g$ Fock state.

C. Gauss' law

In Coulomb gauge the equation of motion for A^0 (Gauss' law)

$$\frac{\delta \mathcal{S}_{QED}}{\delta A^0(t,\boldsymbol{x})} = -\boldsymbol{\nabla}^2 A^0(t,\boldsymbol{x}) - e\,\psi^\dagger\psi(t,\boldsymbol{x}) = 0 \tag{1}$$

$$A^0(t,\boldsymbol{x}) = \int d\boldsymbol{y}\,\frac{e}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\,\psi^\dagger\psi(t,\boldsymbol{y}) \tag{2}$$

is an operator relation which expresses A^0 non-locally in terms of the electron field $\psi^\dagger\psi$. It implies an instantaneous interaction between electrons, the familiar Coulomb potential $-\alpha/r$. Acting on the vacuum, $A^0\,|0\rangle$ can create an e^-e^+ pair. However, care is required due to the Dirac constraints of Coulomb gauge [11].

Gauss' law (1) is not an equation of motion in temporal gauge since $A^0(t,\boldsymbol{x}) = 0$ is fixed. The Coulomb potential is generated in a different way. The condition $A^0(t,\boldsymbol{x}) = 0$ does not fully fix the gauge, allowing time independent gauge transformations [10]. Those transformations are generated by Gauss' operator, the lhs. of (1) which is not required to vanish in temporal gauge,

$$\frac{\delta \mathcal{S}_{QED}}{\delta A^0(t,\boldsymbol{x})} \equiv \mathcal{G}(t,\boldsymbol{x}) = \boldsymbol{\nabla}\cdot\boldsymbol{E}(t,\boldsymbol{x}) - e\,\psi^\dagger\psi(t,\boldsymbol{x}) \tag{3}$$

The electric field $\boldsymbol{E}$ is conjugate to $-\boldsymbol{A}$, so the equal-time commutation relations are

$$\big[E^j(t,\boldsymbol{x}), A^k(t,\boldsymbol{y})\big] = i\,\delta^{jk}\delta(\boldsymbol{x}-\boldsymbol{y}) \qquad\qquad \big\{\psi_\alpha^\dagger(t,\boldsymbol{x}), \psi_\beta(t,\boldsymbol{y})\big\} = \delta_{\alpha\beta}\,\delta(\boldsymbol{x}-\boldsymbol{y}) \tag{4}$$

$\mathcal{G}(t,\boldsymbol{x}) = 0$ cannot be imposed as an operator condition (valid for all states), as this would be incompatible with the commutation relations (4). Instead, Gauss' law is implemented as a *constraint on physical states*,

$$\mathcal{G}(t,\boldsymbol{x})\,|phys\rangle = \big[\boldsymbol{\nabla}\cdot\boldsymbol{E}(t,\boldsymbol{x}) - e\,\psi^\dagger\psi(t,\boldsymbol{x})\big]\,|phys\rangle = 0 \tag{5}$$

This ensures that $|phys\rangle$ states are invariant under the time independent gauge transformations generated by $\mathcal{G}(t,\boldsymbol{x})$. Gauss' operator commutes with the Hamiltonian, $[\mathcal{G}(t,\boldsymbol{x}), H(t)] = 0$, so if (5) is imposed at any time t (and all $\boldsymbol{x}$) then it will hold at all times.[1] [2]

This discussion for QED applies with straightforward modifications also to QCD.

D. Local instantaneous interactions

In temporal gauge the standard QFT methods of equal time canonical quantization applies. The Poincaré generators, *i.e.*, the translation, rotation and boost generators, can be derived from the action and are local in spacetime. It is instructive to consider how the non-local Coulomb potential $-\alpha/r$ arises in Positronium atoms.

Consider the rest frame Positronium state at $t = 0$ in temporal gauge,

$$\big|e^-e^+\big\rangle = \int d\boldsymbol{x}_1 d\boldsymbol{x}_2\,\bar\psi_\alpha(\boldsymbol{x}_1) W[\boldsymbol{A}]\Phi_{\alpha\beta}(\boldsymbol{x}_1-\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_2)\,|0\rangle \tag{6}$$

$$W[\boldsymbol{A}] = \exp\Big[\frac{ie}{4\pi}\int d^3\boldsymbol{y}\,\boldsymbol{A}(\boldsymbol{y})\cdot\boldsymbol{\nabla}_y\Big(\frac{1}{|\boldsymbol{y}-\boldsymbol{x}_1|} - \frac{1}{|\boldsymbol{y}-\boldsymbol{x}_2|}\Big)\Big] \tag{7}$$

$\bar\psi(\boldsymbol{x}_1)$ creates an electron at $\boldsymbol{x}_1$ and $\psi(\boldsymbol{x}_2)$ a positron at $\boldsymbol{x}_2$, distributed according to the c-numbered wave function $\Phi(\boldsymbol{x}_1-\boldsymbol{x}_2)$. The gauge field functional $W[\boldsymbol{A}]$ is required for $|e^-e^+\rangle$ to satisfy Gauss' constraint (5) (see below). The (longitudinal) gauge field operators $\boldsymbol{A}(\boldsymbol{y})$ mutually commute at $t = 0$, $\big[A^j(\boldsymbol{x}), A^k(\boldsymbol{y})\big] = 0$. Hence there is (in QED) no need to specify an operator ordering in (7).

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[1] If we set $\boldsymbol{E} = -\boldsymbol{\nabla}A^0$ then Gauss' constraint (5) would look like Gauss' law (1), but applied only to gauge invariant states.

[2] The rules of temporal gauge may explain a puzzling feature of hadrons. The hadron spectrum suggests that their valence states ($|q\bar q\rangle$, $|qqq\rangle$) dominate, yet the quarks are strongly bound. Why does the color field not create a multitude of gluons and $q\bar q$ pairs, *i.e.*, how is it possible that the valence Fock states are dominant? Given that the ground state $|0\rangle$ is physical, $\mathcal{G}(t,\boldsymbol{x})\,|0\rangle = 0$, so the operators in $\mathcal{G}$ do not create particles from the vacuum, but they do provide binding.

Using the commutation relations (4) at $t = 0$ and recalling that $\boldsymbol{\nabla}_x^2\, |\boldsymbol{x}-\boldsymbol{y}|^{-1} = -4\pi\,\delta^3(\boldsymbol{x}-\boldsymbol{y})$,

$$[\boldsymbol{\nabla}\cdot\boldsymbol{E}(\boldsymbol{x}), W[\boldsymbol{A}]] = \frac{i^2 e}{4\pi}\,\partial_j^x \int d^3\boldsymbol{y}\,\delta^3(\boldsymbol{x}-\boldsymbol{y})\partial_j^y\Big(\frac{1}{|\boldsymbol{y}-\boldsymbol{x}_1|}-\frac{1}{|\boldsymbol{y}-\boldsymbol{x}_2|}\Big)W[\boldsymbol{A}] = -\frac{e}{4\pi}\boldsymbol{\nabla}_x^2\Big(\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_1|}-\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_2|}\Big)W[\boldsymbol{A}]$$
$$= e\left[\delta^3(\boldsymbol{x}-\boldsymbol{x}_1)-\delta^3(\boldsymbol{x}-\boldsymbol{x}_2)\right]W[\boldsymbol{A}] \tag{8}$$

This cancels the $\psi^\dagger\psi$ contribution in (5),

$$\left[-e\psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{x}), \bar\psi_\alpha(\boldsymbol{x}_1)\psi_\beta(\boldsymbol{x}_2)\right] = -e\left[\delta^3(\boldsymbol{x}-\boldsymbol{x}_1)-\delta^3(\boldsymbol{x}-\boldsymbol{x}_2)\right]\bar\psi_\alpha(\boldsymbol{x}_1)\psi_\beta(\boldsymbol{x}_2) \tag{9}$$

Thus for a gauge invariant vacuum, $\mathcal{G}(t,\boldsymbol{x})\,|0\rangle = 0$, the Positronium state $|e^-e^+\rangle$ satisfies Gauss' constraint (5).

The QED Hamiltonian in temporal gauge is

$$H(t=0) = \int d\boldsymbol{x}\Big\{\tfrac{1}{2}\boldsymbol{E}(\boldsymbol{x})^2 + \tfrac{1}{4}F^{jk}F^{jk}(\boldsymbol{x}) + \bar\psi(\boldsymbol{x})\big[-i\gamma^j\overrightarrow{\partial}_j + m - e\gamma^j A^j(\boldsymbol{x})\big]\psi(\boldsymbol{x})\big]\Big\} \tag{10}$$

Since $|e^-e^+\rangle$ has only longitudinal photons the transverse photon kinetic energy term $\frac{1}{4}F^{jk}F^{jk}(\boldsymbol{x})$ does not contribute to $H\,|e^-e^+\rangle$. For non-relativistic Positronium we may at lowest order (Schrödinger equation) neglect the interaction term $-e\,\bar\psi\gamma^j A^j\psi$. Taking the photon field energy density to vanish for the vacuum, $\frac{1}{2}\boldsymbol{E}^2(\boldsymbol{x})\,|0\rangle = 0$, it contributes only through commutators with $W[\boldsymbol{A}]$,

$$\big[E^j(\boldsymbol{x}), W[\boldsymbol{A}]\big] = \frac{i^2 e}{4\pi}\,\partial_j^x\Big(\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_1|}-\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_2|}\Big)W[\boldsymbol{A}]$$
$$\big[E^j(\boldsymbol{x}), \big[E^j(\boldsymbol{x}), W[\boldsymbol{A}]\big]\big] = \frac{i^4 e^2}{(4\pi)^2}\Big[\partial_j^x\Big(\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_1|}-\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_2|}\Big)\Big]^2 W[\boldsymbol{A}]$$
$$\int d\boldsymbol{x}\,\big[\tfrac{1}{2}\boldsymbol{E}^2(\boldsymbol{x}), W[\boldsymbol{A}]\big] = \frac{-e^2}{2(4\pi)^2}\int d\boldsymbol{x}\Big(\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_1|}-\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_2|}\Big)\boldsymbol{\nabla}^2\Big(\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_1|}-\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_2|}\Big)W[\boldsymbol{A}]$$
$$= \frac{e^2}{2(4\pi)}\Big(-\frac{1}{|\boldsymbol{x}_1-\boldsymbol{x}_2|}-\frac{1}{|\boldsymbol{x}_1-\boldsymbol{x}_2|}+\frac{2}{0}\Big)W[\boldsymbol{A}] = -\frac{\alpha}{|\boldsymbol{x}_1-\boldsymbol{x}_2|}W[\boldsymbol{A}] \tag{11}$$

In the last step I neglected infinite but $\boldsymbol{x}_1, \boldsymbol{x}_2$ independent contributions. Hence the result is the (negative) Coulomb potential, even though $\frac{1}{2}\boldsymbol{E}^2$ is a positive definite operator.

Including the electron kinetic energy contribution $\int d\boldsymbol{x}\,\bar\psi(\boldsymbol{x})\big[-i\gamma^j\overrightarrow{\partial}_j + m\big]\psi(\boldsymbol{x})$ in (10) the eigenstate condition $H\,|e^-e^+\rangle = (2m + E_b)\,|e^-e^+\rangle$ gives (in the non-relativistic limit) the Schrödinger equation for $\Phi_{\alpha\beta}(\boldsymbol{x}_1-\boldsymbol{x}_2)$, where E_b is the binding energy.

E. Lessons

The Hamiltonian (10) is obtained in a standard way [11] from the energy-momentum tensor of QED. The states need to have a gauge link between the charges in order to satisfy Gauss' constraint (5). The functional $W[\boldsymbol{A}]$ in (6) may be viewed as a sum over gauge links, arranged along the field lines. Its commutator with the Hamiltonian gives the electric field energy, which equals the Coulomb potential when the (infinite) electron self-energies are subtracted.

This is a straightforward derivation of the Schrödinger equation from the QED action. As such it may serve as an introduction to field theory methods, building on previous experience with the Hydrogen atom in quantum mechanics. In particular, it illustrates how the instantaneous Coulomb potential arises due to the local gauge invariance of QED.

Gauss' constraint (5) may be viewed as a differential equation for the longitudinal electric field $\boldsymbol{E}_L$ acting on $|phys\rangle$, with the solution

$$\boldsymbol{E}_L(\boldsymbol{x})\,|phys\rangle = -\boldsymbol{\nabla}_x\int d\boldsymbol{y}\,\frac{e}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\,\psi^\dagger\psi(\boldsymbol{y})\,|phys\rangle \tag{12}$$

This is closely analogous to (2) in Coulomb gauge. QCD differs from QED in that color singlet states do not generate a color octet field $\boldsymbol{E}_L^a$. Each color component of a Fock state generates an octet field, but the fields cancel in the sum over Fock state colors. This allows to consider boundary conditions on the octet fields which (unlike in (12)) do not vanish at spatial infinity. Equivalently, a homogeneous solution may be added to (12).

There is a unique homogeneous solution which preserves rotational and space translation symmetry. It gives rise to a spatially isotropic gauge field energy density in the vacuum, whose magnitude must be the same for all Fock states. This implies a universal scale (Λ_{QCD}) and adds a linear component to the instantaneous potential of $q\bar{q}$ states. Analogous confining potentials are implied for qqq, $q\bar{q}g$ and gg color singlet states. Since the scale is introduced via a boundary condition the Poincaré invariance of the action can be preserved [7–9].

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