"But there is no Hamiltonian"

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According to Quantum Mechanics, a physical system is described by a Hilbert space with a distinguished self-adjoint operator called Hamiltonian that describes the dynamics.

QED is a quantum theory, so one could expect this kind of a description. Unfortunately, the situation seems to be problematic. In particular, in the context of QED the word Hamiltonian can have many meanings:

1. The QED Hamiltonian: Suppose QED existed nonperturbatively in the sense of some reasonable axioms of Quantum Field Theory, such as the Wightman and the Haag-Kastler axioms. One of "primitive concepts" of these axioms is a strongly continuous unitary representation of the Poincaré group. In particular, we have the self-adjoint generator of time translations – the Hamiltonian. Unfortunately, one can doubt whether QED exists in the sense of these axioms.

Even if the QED Hamiltonian existed, it would be difficult to descibe. It would be an unbounded self-adjoint operator in a strange Hilbert space with a strange domain. An attempt to describe it in the 2nd quantized formalism would almost certainly lead to ill-defined expressions and parameters that have to be renormalized.

This is a common phenomenon. An ill-defined expression, after an appropriate renormalization procedure may lead to a perfectly well-defined self-adjoint operator. There are quite a number of instructive examples in nonrelativistic quantum physics, eg. the delta potential in dimension 2 and 3.

2. The Fundamental Hamiltonian of Theory of Everything: the self-adjoint generator of the evolution in the "Theory of Everything", which is known only to the God. One can doubt whether humans will ever learn it. Maybe it exists. Maybe not – in reality the laws of nature may be very different from our naive ideas. In any case, it is beyond QED, which is too narrow to describe Everything.

3. The formal QED Hamiltonian: We try to write a formal expression for the QED Hamiltonian in terms of quantum fields, which satisfies fundamental symmetries of the theory, in particular the Lorentz symmetry. As indicated above, we should not be surprised if some parameters entering the expression are ill defined and have to be renormalized. Besides, we should probably add appropriate counterterms and it could be difficult to guess them.

Anyway, we do not care much about whether the formal expression corresponds to a self-adjoint operator or not. In reality, it probably does not.

This type of a Hamiltonian is quite common in the literature, eg. in the old paper by Sucher and the review article of Shabaev. It can be heuristically used to derive Feynman rules in low orders. It is however safer to use the Lagrangian approach, where it is easier to maintain the Poincaré covariance.

4. Cutoff Hamiltonians: We take the formal QED Hamiltonian and apply a cutoff for large momenta. This may yield a well-defined self-adjoint opertator. One can expect that this approximates the true theory – however, this is only a rough approximation, which should not be taken too seriously. There are quite a number of mathematical works about this cutoff Hamiltonian, especially with the matter described by a nonrelativistic expression. It is sometimes called by the name of the Pauli-Fierz Hamiltonian, which is historically not quite correct.

5. Effective Hamiltonians: Operators used for approximate computations of various physical and chemical quantities, especially, bound state energies. They may have more or less convincing justifications. They are often partly based on empirical evidence. They are suitable only for some restricted classes of problems.

   Examples include

   (a) the no-pair Dirac-Coulomb Hamiltonian,

   (b) the no-pair Dirac-Coulomb Hamiltonian with the Breit term.

So what is the main object of Quantum Field Theory (according to physicists, not mathematicians), if it is not a Hamiltonian? Most textbooks are not very clear about this point.

One possible answer, stated eg. in Itzykson-Zuber, is the following: The basic concept of QFT is the collection of (time-ordered) n-point (Green) functions.

Another favorite object of contemporary high energy physicists, which they often treat as the basic concept of a quantum field theory, is the effective action. Formally, differentiating the effective action and performing simple algebraic operations we obtain Green's functions. Therefore, the collection of Green's functions can be treated as an object equivalent to the effective action (unless we worry about problems with its differentiability).

It is likely that some regularized versions of QED exist nonperturbatively. (Even this is an optimistic statement, at least in the case of the usual regularization schemes such as Pauli-Villars). Obviously, they depend on the cutoff parameter and the regularization scheme and they probably do not converge to a nontrivial limit as the cutoff parameter goes to infinity.

However, one can expect that for a fixed energy this dependence is very weak for a very big range of large cutoff parameters. Therefore, for practical purposes and bounded energies one can perhaps view QED as defined nonperturbatively. This definition does not involve a Hamiltonian in a Hilbert space. It gives a prescription how to compute Green's functions or the effective action.

Effective Hamiltonians

Let me try to describe an abstract theory of effective Hamiltonians. I will mostly follow the analysis of V.Shabaev (who attributes it to Fojas-Nagy and Kato).

I will describe two kinds of effective Hamiltonians, one sums up the Brillouin-Wigner perturbation theory, the other is related to the Raileigh-Schrödinger perturbation theory.

Suppose a physical system is described by a (huge) Hilbert space $\mathcal{H}$. The dynamics is described by a (poorly known) Hamiltonian H.

Inside $\mathcal{H}$ we have a (relatively small) subspace $\mathcal{H}_0$, which is well understood. We will actually assume that it is finite dimensional. We can write

$$H = \begin{bmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{bmatrix}.$$

Suppose that the initial state belongs to $\mathcal{H}_0$ and we can measure the final state if it falls into $\mathcal{H}_0$. The probability of a measurement is the square of the absolute value of the corresponding amplitude:

$$(\Psi_+|\mathrm{e}^{-\mathrm{i}tH}\Psi_-), \quad \Psi_+, \Psi_- \in \mathcal{H}_0.$$

Measurable quantities can be described by the Laplace transform of the expectation vales

$$-\mathrm{i}\int_0^\infty (\Psi_+|\mathrm{e}^{-\mathrm{i}tH}\Psi_-)\mathrm{e}^{\mathrm{i}tE}\mathrm{d}t \;=\; \big(\Psi_+|(E\mathbb{1}-H)^{-1}\Psi_-\big).$$

where $\mathrm{Im}E > 0$.

Now

$$\big(\Psi_+|(E\mathbb{1}-H)^{-1}\Psi_-\big) \;=\; \big(\Psi_+|(E\mathbb{1}_0-H_{\rm BW}(E))^{-1}\Psi_-\big),$$

where

$$H_{\rm BW}(E) := H_{00}-H_{01}(E\mathbb{1}_1-H_{11})^{-1}H_{10}$$

can be called the Brillouin-Wigner effective Hamiltonian and is an energy dependent operator on the small space $\mathcal{H}_0$. It contains complete physical information about the subsystem described by $\mathcal{H}_0$. We do not need to know whether it is derived from a Hamiltonian on a bigger space!

Assume that the spectrum of (the big) H is absolutely continuous. Then (1) can often be extended accross the real axis in E. Singularities of (1) will be called bound state energies. They are solutions of

$$\det\left(E\mathbb{1}_0 - H_{\mathrm{BW}}(E)\right) = 0. \qquad (1)$$

Assume that off-diagonal elements of H are small. Then bound state energies are close to the eigenvalues of H_{00} and are usually simple poles, so that

$$\left(E\mathbb{1}_0 - H_{\mathrm{BW}}(E)\right)^{-1} = \sum_i P_i (E - E_i)^{-1}.$$

(E_i do not have to be real and P_i do not have to be idempotents!).

Let us show an example how one computes with an effective hamiltonian H_{BW}.

Suppose that

$$H_{\mathrm{BW}}(\alpha, E) = H_0 + \alpha V_1^{\mathrm{eff}}(E) + \alpha^2 V_2^{\mathrm{eff}}(E) + \dots,$$

Let E_0 be a simple eigenvalue of H_0 with the eigenvaector Ψ_0. Then (1) yields the following perturbed bound state energy:

$$E(\alpha) = E_0 + \alpha E_1 + \alpha^2 E_2 + \dots$$

where

$$
\begin{aligned}
E_1 &= \langle V_1^{\rm eff}(E_0)\rangle, \\
E_2 &= \langle V_2^{\rm eff}(E_0)\rangle + \langle V_1^{\rm eff}(E_0)\rangle \partial_E \langle V_1^{\rm eff}(E_0)\rangle \\
&\quad + \langle V_1^{\rm eff}(E_0)\big(\mathbb{1} - P_0\big)(E_0 - H_0)^{-1} V_1^{\rm eff}(E_0)\rangle.
\end{aligned}
$$

Here

$$
\langle V_1^{\rm eff}(E_0)\rangle := (\Psi_0|A\Psi_0), \quad P_0 := |\Psi_0)(\Psi_0|.
$$

$H_{\mathrm{BW}}(E)$ depends on the energy. One can (in a unique way!) introduce a different effective Hamiltonian, which does not depend on the energy and gives the same energy levels $\{E_1, E_2, \dots\}$.

First note that

$$P_i := \oint_{\Gamma_i} \big(E\mathbb{1} - H_{\mathrm{BW}}(E)\big)^{-1} \mathrm{d}E,$$

where Γ_i encircles E_i.

Choose a contour Γ that encircles $\{E_1, E_2, \dots\}$ and set

$$P = \oint_\Gamma \big(E\mathbb{1} - H_{\mathrm{BW}}(E)\big)^{-1} \mathrm{d}E = \sum_i P_i,$$

$$K = \oint_\Gamma E\big(E\mathbb{1} - H_{\mathrm{BW}}(E)\big)^{-1} \mathrm{d}E = \sum_i E_i P_i.$$

Remember that we assumed that the off-diagonal term in H is small. Therefore P is close to the identity and we can define

$$P^{-\frac{1}{2}} = \big(\mathbb{1} + (P - \mathbb{1})\big)^{-\frac{1}{2}}$$

by a power series.

We expect that the rank of P_i equals the dimension of the corresponding eigenvalues of H_{00}, say $\dim P_i = d_i$, where $d_1 + \ldots d_n = \dim \mathcal{H}_0$. Therefore, the range of $K - EP$ has dimension $\dim \mathcal{H}_0 - d_i$ whenever $E = E_i$. Consequently, $\{E_1, E_2, \ldots\}$ are solutions of

$$\det\big(K - EP\big) = 0.$$

Introduce the Rayleigh-Schrödinger effective Hamiltonian

$$H_{\mathrm{RS}} := P^{-\frac{1}{2}} K P^{-\frac{1}{2}}.$$

Then $\{E_1, E_2, \ldots\}$ are solutions of a true eigenvalue problem

$$\det\big(E - H_{\mathrm{RS}}\big) = 0. \tag{2}$$

Time ordered Green's functions

Suppose that Ω is the ground state of H and

$$\phi[f] = \int \phi(\xi) f(\xi) \mathrm{d}\xi$$

is a family of auxiliary operators called fields, which for simplicity we assume to be self-adjoint. We will write

$$\phi[t, f] := \mathrm{e}^{\mathrm{i}tH} \phi[f] \mathrm{e}^{-\mathrm{i}tH} = \int \phi(t, \xi) f(\xi) \mathrm{d}\xi$$

for these operators in the Heisenberg picture.

The time-ordered Green's functions are defined as

$$\Big(\Omega\Big|\mathrm{T}\big(\phi(t_n,\xi_n)\cdots\phi(t_1,\xi_1)\big)\Omega\Big)$$

One can argue that Green's functions are closely related to measurable quantities. Indeed, suppose the experimentalist can prepare the state Ω in distant past, and he/she can measure Ω in distant future. We also suppose that he/she can perturb the dynamics in a controllable way by adding to the Hamiltonian a field, so that the dynamics is generated by

$$H[f] := H + \phi[f].$$

Thus the relevant amplitudes are

$$\begin{aligned}
&\lim_{t^+,-t^-\to\infty}\left(\Omega\Big|\mathrm{Texp}\Big(-\mathrm{i}\int_{t^-}^{t^+}H[f(t)]\mathrm{d}t\Big)\Omega\right)\\
=&\left(\Omega\Big|\mathrm{Texp}\Big(-\mathrm{i}\int_{-\infty}^{\infty}\phi[t,f(t)]\mathrm{d}t\Big)\Omega\right)\\
=&\sum_{n=0}^{\infty}\frac{(-\mathrm{i})^n}{n!}\int\cdots\int\Big(\Omega\Big|\mathrm{T}\big(\phi(t_n,\xi_n)\cdots\phi(t_1,\xi_1)\big)\Omega\Big)\\
&\qquad\times f(t_n,\xi_n)\cdots f(t_1,\xi_n)\mathrm{d}t_n\mathrm{d}\xi_n\cdots\mathrm{d}t_1\mathrm{d}\xi_1.
\end{aligned}$$

Two-times Green's functions

One can also consider a slightly different picture of a realistic experiment. Let us assume that the space of experimentally accessible states $\mathcal{H}_0$ have the form

$$\Psi_F := \int \int \cdots \int F(\xi_n \ldots, \xi_1)\phi(\xi_n) \cdots \phi(\xi_1)\Omega \mathrm{d}\xi_n \cdots \xi_1$$

for some fixed values of n and some space of functions F.

The corresponding amplitudes

$$\begin{aligned}
&\left(\Psi_{F^+}\middle|\mathrm{e}^{-\mathrm{i}(t^+-t^-)H}\Psi_{F^-}\right)\\
&= \int\dots\int \mathrm{d}\xi_1^+\cdots\mathrm{d}\xi_1^-\,\overline{F^+(\xi_{n^+}^+,\dots,\xi_1^+)}F^-(\xi_{n^-}^-,\dots,\xi_1^-)\\
&\quad\times\left(\Omega\middle|\phi(t^+,\xi_1^+)\cdots\phi(t^+,\xi_{n^+}^+)\phi(t^-,\xi_{n-}^-)\cdots\phi(t^-,\xi_1^-)\Omega\right)
\end{aligned}$$

are expressed in terms of two-times Green's functions. Thus two-times Green's functions can be used to define the Brillouin-Wigner effective Hamiltonian on $\mathcal{H}_0$.

Clearly, two-times Green's functions can be obtained as limits of the usual time-ordered Green's functions.

$$\begin{aligned}
&\Big(\Omega\Big|\phi(t^+,\xi_1^+)\cdots\phi(t^+,\xi_{n^+}^+)\\
&\qquad\times\phi(t^-,\xi_{n-}^-)\cdots\phi(t^-,\xi_1^-)\Omega\Big)\\
=\ &\lim_{\epsilon\searrow 0}\Big(\Omega\Big|\mathrm{T}\big(\phi(t_{1,\epsilon}^+,\xi_1^+)\cdots\phi(t_{n^+,\epsilon}^+,\xi_{n^+}^+)\\
&\qquad\times\phi(t_{n^-,\epsilon}^-,\xi_{n-}^-)\cdots\phi(t_{1,\epsilon}^-,\xi_1^-)\big)\Omega\Big),\\
t_{j,\epsilon}^+ &:= t^+ + \epsilon(n-j),\qquad t_{j,\epsilon}^- := t^- - (n-j)\epsilon.
\end{aligned}$$

Second quantized Hamiltonians

Suppose that the Hamiltonian is expressed in terms of creation/annihilation operators as

$$H = \int \varepsilon(\xi) a^*(\xi) a(\xi) \mathrm{d}\xi + W(a^*, a),$$

where $W(a^*, a)$ is a certain polynomial in creation/annihilation operators. Assume that $\phi(\xi)$ are linear combinations of $a(\xi')$ and $a^*(\xi')$.

Then time ordered Green's functions are given by the so-called Feynman rules as formal sums of evaluations of appropriate diagrams. This is the consequence of a series of classic facts that go under the name of Dyson expansion, Wick's Theorem, Gell-Mann–Low Theorem, Linked Cluster Theorem.

It is natural to treat Green's functions as the basic object of the theory defined by the Feynman rules, and not the Hamiltonian!

Local Quantum Field Theory

Physicists want a theory that satisfies the following requirements:

1. it is Poincaré covariant;
2. the Hamiltonian (the generator os time translations) is bounded from below;
3. it is local (satisfies the Einstein causality);
4. it depends on a finite number of parameters.

The requirements 1.-3. have a fundamental nature.

The requirement 4. is less fundamental and more practical: one wants a theory with a predictive power.

Mathematical physicists tried to formalize 1.-3. with axioms (Wightman, and also Haag-Kastler axioms).

These axioms are rarely mentioned in physics textbooks. Theoretical physicists start from a formal path integral involving a local Lagrangian. Then they use an appropriate propagator in Feynman diagrams. One can argue that this is morally equivalent to adopting the requirements 1.-3.

The requirement 4. leads to renormalizable theories and restricts severely possible Lagrangians.

For interacting theories 1.-3. seem incompatible with Hamiltonians expressed in terms of second quantization. This is due mainly to the ultraviolet problem. One can try to use formal Hamiltonians that are relativistic and local for low momenta, with the momenta larger than Λ suppressed by a cutoff, add appropriate counterterms and tune the bare parameters so that the Green's functions in the limit $\Lambda \to \infty$ exist and have correct symmetries. This is the Hamiltonian approach to renormalization. This approach was tried in the early days of Quantum Field Theory. Nowadays it seems that only some mathematical physicists treat it seriously.

Theoretical physicists have developed a number of techniques to compute perturbatively Green's functions starting from the Lagrangian (Pauli-Villars, dimensional regularization, dispersion relations). These techniques usually cannot be interpreted in terms of a modification of the Hamiltonian. In the end they lead to renormalizable theories. Fortunately, renormalizable theories are very rigid, and no matter which regularization is taken, one seems to obtain the same family of theories.

One can imagine that some of these regularizations make sense nonperturbatively. Thus if r denotes the regularization scheme and Λ the cutoff parameter, for finite Λ we have obtain well defined objects (say, Green's functions), which are analytic in α:

$$G^{r,\Lambda}(\alpha) = \sum_{n=0}^{\infty} \alpha^n G_n^{r,\Lambda}.$$

We do not know whether

$$\lim_{\Lambda \nearrow \infty} G^{r,\Lambda}(\alpha)$$

exists (probably not).

However, the coefficients in the perturbation expansion have well-defined limits that do not depend on the regularization scheme

$$\lim_{\Lambda \nearrow \infty} G_n^{r,\Lambda} = G_n.$$

The final theory is given by a formal power series

$$\sum_{n=0}^{\infty} \alpha^n G_n.$$

The Lagrangian approach breaks as few symmetries of the problem as possible and the choice of counterterms is limited. The Hamiltonian approach breaks manifestly the Lorentz covariance and it is not clear how to choose counterterms. Therefore it is considered to be inferior.

Quantum Electrodynamics

Here are typical terms that appear in the QED Lagrangian:

$$\mathcal{L}_{\text{e.m.}} := -\frac{Z_3}{4}(\partial_\mu A_\nu - \partial_\nu A_\mu)(\partial^\mu A^\nu - \partial^\nu A^\mu) - \frac{\mu_0^2 Z_3}{2} A_\mu A^\mu,$$

$$\mathcal{L}_p := Z_{1,p}\tilde{\psi}_p \gamma_\mu (\mathrm{i}\partial^\mu - e z_p A^\mu)\psi_p - m_{p,0} Z_{1,p}\tilde{\psi}_p \psi_p,$$

$$\begin{aligned}\mathcal{L}_q := & -Z_{1,q}\big((\partial_\mu - \mathrm{i}e z_q A_\mu)\psi_q\big)^*(\partial_\mu - \mathrm{i}e z_q A_\mu)\psi_q \\ & -m_{q,0}^2 Z_{1,q}\psi_q^*\psi_q - \frac{\lambda_{q,0} Z_{1,q}^2}{4}\big(\psi_q^*\psi_q\big)^2.\end{aligned}$$

(We set $\hbar = c = 1$).

$$\mathcal{L} = \mathcal{L}_{\text{e.m.}} + \sum_p \mathcal{L}_p + \sum_q \mathcal{L}_q.$$

p is the name of a species of Dirac fermions. q is the name of a species of charged scalar bosons.

The parameters Z_3, $Z_{1,p}$, $Z_{1,q}$, μ_0, $m_{p,0}$, $m_{q,0}$, $\lambda_{q,0}$ are bare – they need to be renormalized. (μ_0 is introduced to help with the infrared problem). $z_p e$, $z_q e$ are the charges of the particles.

A theory is fixed by specifying the physical masses of all particles (which correspond to the position of the singularity of 2-point Green's functions) and their charges. In addition, for bosons one needs to specify the value of 4-point functions at a certain point – this is related to the λ term.

By Furry's Theorem, QED amplitudes without external photon depend only on even powers of e. Therefore, in practice instead of e one uses the finestructure constant $\alpha = \frac{e^2}{4\pi\hbar c}$.

Unfortunately, QED has to be treated perturbatively. The usual approach, described in every textbook, uses e (or, equivalently, α) as the small parameter. The theory with $e = 0$ corresponds to non-interacting charged particles and photons. Its Green's functions do not have bound states. We will not see bound states in the perturbative treatment either. Fortunately, there are other approaches, where bound states can be seen already at the zeroth approximation.

Nonrelativistic linit of QED

In the nonrelativistic limit of QED we expect to obtain the many-body Schrödinger-Coulomb Hamiltonian of several species of particles.

For each bosonic "relativistic species", we have two "nonrelativistic species" corresponding to particles and antiparticles. For each fermionic "relativistic species" we have four "nonrelativistic species" corresponding to particles and antiparticles, and also to two spin states. Each nonrelativistic species p has the mass m_p and the charge $\pm z_p e$, where the sign is $+$ for particles and $-$ for antiparticles.

The Hamiltonian is the sum of kinetic terms and 2-body interaction terms. For every species p the kinetic term is

$$\frac{1}{2m_p}\int \mathrm{d}\vec{x} a_p^*(\vec{x})(-\Delta)a_p(\vec{x})$$

For every pair of species $p \neq q$ the interaction term is

$$\frac{1}{2}\int \mathrm{d}\vec{x}\int \mathrm{d}\vec{y} a_p^*(\vec{x})a_q^*(\vec{y})\frac{\alpha z_p z_q \mathrm{e}^{-\mu|\vec{x}-\vec{y}|}}{|\vec{x}-\vec{y}|}a_q(\vec{y})a_p(\vec{x}).$$

Clearly, the many-body Schrödinger-Coulomb Hamiltonian is a well defined self-adjoint operator. Its Green's functions are well defined nonperturbatively and one can study rigorously their singularities. They correspond to true bound states and metastable states (resonances) of N-body subsystems.

It is possible (although not easy) to treat Schrödinger-Coulomb Green's functions as the zeroth approximation to QED Green's functions. One can treat $\frac{1}{c}$ as the small parameter. Equivalently, one could use α as the small parameter. e is kept constant.

The development if this approach is attributed to Lepage. It was later applied in QED by Pachucki. This approach is applicable only to systems with small z_p's. For practical reasons, one usually treats only few particle systems. Typical applications include

1. positronium,
2. Hydrogen with nucleus of finite mass,
3. Helium.

QED in external potentials

Suppose that some of the particles are so heavy, that they can be treated just as the sources of the electromagnetic field moving along prescribed trajectories. Then we can use QED with both external and quantized electromagnetic potentials. In the Lagrangian for charged particles we replace eA_μ with $eA_\mu + A^{\rm ext}_\mu$, where $A^{\rm ext}_\mu$ is a prescribed function on spacetime. (Note that there is no small constant e in front of $A^{\rm ext}_\mu$).

Setting $e = 0$, beside independent photons, we obtain independent charged particles in an external potential. The theory of charged particles is quadratic, and hence well understood nonperturbatively. In principle their Green's functions are well defined.

If $A_\mu^{\rm ext}$ is stationary, then singularities of Green's functions correspond to bound states of the (one-body) Dirac/Klein-Gordon Hamiltonian.

Then one can again use e (or α) as the small parameter to add radiative corrections.

One of researchers that uses this approach is Shabaev.

It is used most often to take into account the potential $\frac{Z\alpha}{|\vec{x}|}$ generated by the nucleus. In practice one splits this potential into two parts – one part is treated perturbatively, for the other one uses the Furry picture, which involves changing the vacuum and the propagators. This splitting is to a large extent arbitrary and dictated by practical considerations.

This approach is especially suitable in the case of heavily charged ions such as the Uranium, for which $Z\alpha$ is not a small parameter.