Existence of Solutions to the Maxwell–Schrödinger Equations with a Background Electric Charge

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Outline

1. Introduction: Situation, model, specialisation
2. Conditions for consistency
3. Making the functional explicitly bounded below: removing V
4. Euclidean space with no background charge
5. Existence on compact manifolds
6. Generalisations

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Situation

- Classical collection of N identical charged particles interacting with an electromagnetic field.
- Obvious way to couple these is with minimal coupling of the Klein–Gordon field to the Maxwell gauge field (i.e. replace the derivatives with covariant derivatives):

$$\mathcal{L} = \frac{1}{2m} |D\psi|^2 - \frac{\epsilon_0}{4} F^2.$$

- Less relativistic version of this is the Maxwell–Schrödinger system; of particular interest in describing LASER physics & many other types of light-matter interactions.
- Here, shall consider M–S with an additional background charge. Interesting physically, also sensible mathematically.

Maxwell–Schrödinger Lagrangian

Let Ω be an n-dimensional Riemannian manifold, $A_\mu : \mathbb{R} \times \Omega \to \mathbb{R}$ ($\mu = 0, \ldots, n$), $\psi : \mathbb{R} \times \Omega \to \mathbb{C}$, and $J_\mu = (\rho, \boldsymbol{j})$ a fixed ("background") charge-current. The full Lagrangian of the theory is

$$L = \int_\Omega i\hbar \overline{\psi} D_0 \psi - \frac{1}{2m} \overline{D_i \psi} D^i \psi - \frac{\epsilon_0}{4} F^2 - eA \cdot J,$$

with $D_0 = \partial_0 + iec^{-1} A_0$, $D_i = \nabla_i + iec^{-1} A_i$.

Euler–Lagrange equations

Writing $\psi = u e^{iS}$ with u, S real functions, we obtain the following Euler–Lagrange equations:

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\,\Delta\, u + \left(e A_0 + \frac{1}{2m}\left|\nabla S - e c^{-1} \boldsymbol{A}\right|^2 \right) u &= -\dot{S} u \\
\partial_t (u^2) - \frac{1}{m}\nabla \cdot \left(\left(\nabla S - e c^{-1} \boldsymbol{A} \right) u^2 \right) &= 0 \\
\nabla \cdot \boldsymbol{E} &= \frac{1}{\epsilon_0} e (u^2 + \rho) \\
\nabla (\nabla \cdot \boldsymbol{A}) - \Delta\, \boldsymbol{A} - \frac{1}{c^2} \dot{\boldsymbol{E}} &= \frac{e}{\epsilon_0 c^2} \left(\frac{1}{m} (\nabla S - e c^{-1} \boldsymbol{A}) u^2 + \boldsymbol{j} \right),
\end{aligned}
$$

where $\boldsymbol{E} = -c^{-1} \dot{\boldsymbol{A}} - \nabla A_0$. Then

$$
e \left(u^2, \frac{1}{m} (\nabla S - e c^{-1} \boldsymbol{A}) u^2 \right)
$$

looks like a charge-current vector.

Specialisation: Euler–Lagrange equations

We restrict to electrostatics and stationary states,

$$\boldsymbol{A} = 0, \qquad S = -\omega t, \qquad A_0(t, x) = V(x),$$

and rescale to make most of the constants 1. The remaining nontrivial Euler–Lagrange equations are

$$\begin{aligned} -\frac{1}{2}\,\Delta\, u + eVu &= \omega u \\ -\,\Delta\, V &= e(u^2 + \rho), \end{aligned}$$

the *Schrödinger–Coulomb equations.*

The Schrödinger–Coulomb energy functional

$$-\frac{1}{2}\,\Delta\,u + eVu = \omega u$$
$$-\,\Delta\,V = e(u^2 + \rho)$$

These equations arise as the Euler–Lagrange equations of the following energy functional:

$$H = \int_\Omega \frac{1}{2}(\nabla u)^2 - \frac{1}{2}(\nabla V)^2 + eV(u^2 + \rho),$$

with the condition $\int_\Omega u^2 = N$, a constant.

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Condition on ρ

Gauss's Law:

$$-\Delta V = e(u^2 + \rho)$$

Suppose Ω compact and $\partial\Omega = \emptyset$. Integrate Gauss's Law over Ω:

$$e \int_\Omega u^2 + \rho = -\int_\Omega \Delta V = -\int_{\partial\Omega} \nabla V \cdot dS = 0.$$

So need

$$\int_\Omega \rho = -\int_\Omega u^2 = -N,$$

for consistency.

Bounding H below

$$H = \int_\Omega \frac{1}{2}(\nabla u)^2 - \frac{1}{2}(\nabla V)^2 + eV(u^2 + \rho)$$

For general V, H is not bounded below. If V solves Gauss's Law, however, multiplying by V and integrating gives

$$e\int_\Omega V(u^2+\rho) = -\int_\Omega V\,\Delta\,V = 0 + \int_\Omega (\nabla V)^2;$$

substituting this into H,

$$H = \int_\Omega (\nabla u)^2 + \frac{1}{2}e\int_\Omega (\nabla V)^2 \geqslant 0$$

(H is a sum of squares).

Outline

Integrating out V

Viz., inverting the Laplacian. On $\mathbb{R}^n$, we know how to do this. On compact manifolds, the argument is more subtle.

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Lemma

On a compact manifold without boundary, a continuous harmonic function is constant.

Therefore $\ker(-\Delta)$ is precisely the constant functions. So if we choose the subset of functions with $\int_\Omega f = 0$, the Laplacian is invertible, and we can write unambiguously

$$V(x) = e[(-\Delta)^{-1}(u^2 + \rho)](x) = e\int_\Omega G(x;y)(u^2 + \rho)(y)\,dy,$$

$G(x;y)$ being the fundamental solution ("Green's function").

The well-defined functional

$$V = e(-\Delta)^{-1}(u^2 + \rho)$$

Inserting this expression for V,

$$\begin{aligned} E[u] &= \int_\Omega (\nabla u)^2 + \frac{1}{2} e \int_\Omega (u^2 + \rho) V \\ &= \int_\Omega (\nabla u)^2 + \frac{1}{2} e^2 \int_\Omega (u^2 + \rho)(-\Delta)^{-1}(u^2 + \rho) \\ &=: T[u] + \frac{1}{2} e^2 J[u^2 + \rho] \end{aligned}$$

There is explicit self-interaction: the Schrödinger equation is nonlinear,

$$-\frac{1}{2}\Delta u + e^2 \left((-\Delta)^{-1}(u^2 + \rho)\right) u = \omega u.$$

(Notice the equations are now also nonlocal.)

Outline

$\mathbb{R}^n$ with $\rho = 0$

Write $u_\lambda = \lambda^{n/2} u(\lambda x)$. Easy to check that $\int_\Omega u_\lambda^2 = \int_\Omega u^2 = N$, say. The terms in the energy scale as:

$$T[u_\lambda] = \lambda^2 T[u]$$
$$J[u_\lambda^2] = \begin{cases} \lambda^{n-2} J[u^2] & n \neq 2 \\ J[u^2] + N^2 \log \lambda & n = 2. \end{cases}$$

Then is easy to check that decreasing λ decreases E. Therefore there is certainly no stable bound state.
(One can do a more careful argument with $\frac{d}{dt}\langle x^2 \rangle$ and so on.)

Outline

How do we make certain the energy integral is finite?

- Write $\|v\|_p = \left(\int_\Omega |v|^p\right)^{1/p}$. $L^p(\Omega) = \{v : \|v\|_p < \infty\}$.
- $T[u] < \infty$ and $\|u\|_2^2 = N \implies u, \nabla u \in L^2(\Omega)$. Write as $u \in H^1(\Omega)$. This space has norm $\|v\|_{H^1}^2 = \|v\|_2^2 + \|\nabla v\|_2^2$.
- $J = J[u^2, u^2] + 2J[u^2, \rho] + J[\rho, \rho]$ more tricky. Sobolev embedding gives $u \in L^p(\Omega)$ for $p < 2^* = 2n/(n-2)$.
  - $J[u^2, \rho]$ gives a condition on ρ using Young's inequality. Find ρ must be in $L^q(\Omega)$ for $2n/(n+2) \leqslant q \leqslant 2$.
  - To bound $J[u^2, u^2]$, also need $n \leqslant 5$, or the Sobolev embedding does not give enough control over the p-norm of u to counteract the singularity of the inverse Laplacian on the diagonal. (So higher dimensions need more conditions on u.)

Existence on compact manifolds: method of proof

1. E is bounded below on $H^1(\Omega)$, therefore it has an infimum, e_0. Take a sequence $u_n \in H^1$ with $E[u_n] \to e_0$.
   (a) $E[u_n]$ is bounded above. $E[u_n] \geqslant \|u_n\|_{H^1} - N$, so the sequence is bounded in H^1.
   (b) The Banach–Alaoglu theorem implies that bounded sequences in Banach spaces have a weakly convergent subsequence, $u_{n_k} \rightharpoonup u$.

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2. Need to show $E[u] = e_0$.
   (a) $E[u] \geqslant e_0$ since $u \in H^1$.
   (b) Other direction: show that E is weakly lower-semicontinuous, which says that $\liminf_{n\to\infty} E[u_n] \geqslant E[u]$. (Done using Sobolev and Young inequalities.) Hence $E[u] = e_0$.

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3. Need to show that $\|u\|_2^2 = N = \lim_{n\to\infty} \|u_n\|_2^2$.
   (a) Equivalent to showing that $\left\|u_{n_k} - u\right\|_2 \to 0$ (*strong convergence in* L^2).
   (b) Rellich–Kondrashov: bounded in H^1 implies that there is a subsequence that does this, $u_{n_{k_j}} \to v$.
   (c) Can show $u = v$ using Cauchy–Schwarz.

Existence on compact manifolds: conclusion

1. E is bounded below on $H^1(\Omega)$, therefore it has an infimum, e_0. Take a sequence $u_n \in H^1$ with $E[u_n] \to e_0$. This sequence has a weakly convergent subsequence $u_{n_k} \rightharpoonup u$.
2. $E[u] = e_0$, by e_0 being an infimum and showing that E is weakly lower-semicontinuous.
3. $\|u\|_2^2 = N = \lim_{n\to\infty} \|u_{n_k}\|_2^2$, because there is a subsequence $u_{n_{k_j}} \to u$ strongly in L^2.
4. Therefore u has total charge Ne, and minimises E. Therefore it also satisfies the Euler–Lagrange equations, and we have shown a solution exists.

Outline

Generalisations

- The result can in theory be joined to one of Benci and Fortunato (a compact 3-dimensional flat manifold with a boundary, with the potential determined on the boundary).
- $n = 6$ may be possible, but the Hamiltonian may have to be modified to do so.
- $\mathbb{R}^n$. Currently working on this. Difficulty lies in choosing the correct space to allow for the energy to be finite, while at the same time bounding the norm in this space so that u_n converges strongly.
- Should not need the manifold to be smooth. (C^2 should be sufficient.)
- Coclite and Georgiev have considered a hydrogenoid potential Zr^{-1} in 3 dimensions (i.e. one generated by a point charge), which gives bound states for atoms with one electron.
- Maxwell–Klein–Gordon in general is much harder, because the natural space on which it is formulated is a Lorentzian manifold, which complicates matters considerably.