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

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0 Preamble

I shall discuss the Maxwell–Schrödinger equations. These are a non-relativistic version of the Maxwell–Klein–Gordon system, the usual method of coupling a scalar field to an electromagnetic field. The plan is as follows:

- First I shall explain the origins of the model, then discuss the specialisation I am talking about today.
- Then I shall discuss some conditions that are required for the equations to be consistent and the energy to be bounded below;
- after which I shall explain how to remove the apparent indefiniteness of the energy by removing one of the fields,
- then an example of why having a nonzero background is likely to be a sensible choice, on non-compact manifolds.
- Then I shall explain the method of proof of existence in a special,
- and then lastly some possible generalisations of this result to more complicated or more general situations, in addition to some other people's work.

We start by setting up the model.

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1 Introduction: Situation, model, specialisation

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

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

A less relativistic version of this is the Maxwell–Schrödinger system; this is of particular interest in describing LASER physics, or indeed, many other types of light-matter interactions (With enough particles that quantum effects such as spin are insignificant).

I shall consider this system with an additional coupling to a background charge, such as the fixed lattice of a metal or a heavy atom: we shall see that this is a sensible thing to do mathematically, as well as interesting physically.

So, the my initial setup looks like this:

Let the space we are considering be a Riemannian manifold Ω (the time dimension is separate, so the actual spacetime is $\mathbb{R}\times\Omega$. Then the wavefunction ψ and the gauge field A_μ are functions on this space, and the Lagrangian looks like this, the terms being:

time derivatives,	rest of Klein–Gordon term,	electromagnetic Lagrangian,	extra background term

Notice again that these are covariant derivatives, including both coupling to the gauge field and taking into account the Riemannian structure on the manifold. (Likewise, the integral is with respect to the measure induced by the metric, &c.)

We are looking for stationary points of the Lagrangian, so we look at the Euler–Lagrange equations associated to it:

Notice first that I have made a polar substitution $\psi = ue^{iS}$; this just makes everything real.

Bearing in mind this comment <at the bottom>, the equations look like:

- A Schrödinger equation, a continuity equation for a charge–current, Gauss's Law, and Ampère's Law.

Now, I wish to specialise to the electrostatic case, with stationary states. (This being the simplest case.)

To do this consistently I take these equations and drop the vector potential, make the scalar potential time-independent and the phase function S just a linear function of time,

which leads to these equations. (Notice I have also rescaled away most of the constants)

- A Schrödinger equation

- and Gauss's Law;

these are called the Schrödinger–Coulomb equations. In this talk I shall describe how to prove they have a solution.

Global study of these equations is most easily done by thinking of them as the Euler–Lagrange equations of an energy functional; the appropriate functional in this case is:

Notice that the ω has become essentially a Lagrange multiplier for condition that the total charge of u is a constant—that's what this condition is, recalling that eu^2 is a charge density.

The other important feature is this minus sign in front of the gradient of V—this means that for general V, the energy functional is not bounded below, which makes minimising it implausible.

I shall now explain some properties of this functional and its Euler–Lagrange equations which we should be aware of before we study it further.

In particular, a condition for ρ that we require in order for the equations to be consistent on a compact manifold with empty boundary; this shall be the case I discuss in detail later.

2 Conditions for consistency

If we integrate Gauss's Law, we obtain this equation; this second equality is using Stokes's Theorem, and it is equal to zero because the boundary is empty.

Therefore, the condition on the total charge implies that ρ has integral $-N$, so that in fact the total charge on the manifold is zero.

Now we ought to see what we actually know about the energy that means it really does turn out to be bounded below.

If we multiply Gauss's Law by V and integrate, we find this equation: integrating by parts, we find this (The zero is the integral over the empty boundary), and then if we substitute this into the energy, we notice it is a sum of squares, and so is bounded below by zero.

Therefore, we would like to get rid of V: it is completely determined by Gauss's Law, and keeping it around makes the functional look more badly-behaved that it necessarily is.

We shall therefore remove it by "solving" for it in the Gauss's Law equation.

3 Making the functional explicitly bounded below: removing V

Therefore we need to invert the Laplacian. We understand how to do this on, for example, $\mathbb{R}^n$, but on compact manifolds, the charge neutrality condition we just discussed makes the issue more subtle (in physics terms, it is inconsistent to try and find the Green's function for Laplace's equation by solving Poisson's equation with just a δ on the right-hand side, since its integral is not zero). Therefore we shall adopt a more nuanced argument.

We shall use the following Lemma:

I assert that this is obvious. Therefore the kernel of the Laplacian as a linear map is only the constant functions, so specifying integral zero is equivalent to quotienting by the kernel, and since a linear operator mapping the quotient of its domain by its kernel to its range is bijective onto its image, the Laplacian has an inverse.

So we can write V as a linear operator acting on $u^2+\rho$; this is actually an integral using the fundamental solution.

If we substitute this into the Hamiltonian from before, we get this expression. (In fact the inverse Laplacian here is a positive operator, so once again we get positivity.)

The Schrödinger equation, which did not originally look nonlinear, is now both nonlinear and nonlocal.

We shall work with this particular energy functional from now on. I define the kinetic term to be T and the Coulomb energy term to be J; we shall now look at a property they possess that suggests that having a nonzero background is of interest in other cases.

In particular, let's look at $\mathbb{R}^n$, with no background.

4 Euclidean space with no background charge

Suppose we look at scaling the coordinates, which amounts to allowing u to spread out a bit. We find that this expression, u_λ, has the same square-integral as u.

If we look at the scaling of the terms in the energy, we find the kinetic term goes like this, and the Coulomb term like this (this anomalous log is present because the inverse of the two-dimensional Laplacian contains a log).

Either way, we see that spreading u out a bit by making λ a bit smaller than one decreases both of these terms in any number of dimensions. Therefore it decreases the energy, so even if u was a bound state, it would not be stable.

In fact, one can do better by looking at this, the change in the spread of u with time, and so on, but that's beyond the scope of this talk.

So having convinced ourselves that we have the right energy functional and do want a background charge, let's discuss how to do the existence proof, at least for compact manifolds.

Recall that if a function minimises the energy, it satisfies the Euler–Lagrange equations. Therefore if we can prove that the energy functional is minimised by u, u will be a solution of the Euler–Lagrange equations.

Firstly, however, we should know where the energy is finite, so we know in what space the function is meaningful, and so it makes sense to minimise it.

5 Existence on compact manifolds

I shall now define a (very small) number of function spaces, all of which are determined, as one might imagine, by the finiteness of integrals.

L^p is simply the functions on the manifold that have their pth power integrable (that's this). It has a norm determined by this integral.

Now, we need the derivative of u to be square-integrable for the kinetic energy to be finite, and we already know that u is square-integrable, because we specified that the total charge is finite; both of these conditions together give us a space called H^1, with this as the obvious norm.

The other term in the energy, J, is slightly harder: it basically contains three functions: u, ρ, and the Green's function. The control H^1 gives us over u's derivative gives (via something called the Sobolev embedding) control over some higher powers of u. This, along with an inequality for convolutions called Young's inequality, allows us to determine (via the cross term between u^2 and ρ) the minimum amount of control we can have over ρ.

However, the term that contains both u^2s, together with the behaviour of the Green's function near the diagonal, gives us an upper limit on the number of dimensions we can talk about: more that five requires that we have more control over u than it just being in H^1.

Therefore we know where our functions can live, so we can now discuss how to show that for a u in H^1, with total charge Ne, the energy is minimised (and hence the Euler–Lagrange equations are satisfied).

Firstly, we know that the energy functional is bounded below (since we spent a great deal of time showing this to be the case earlier); therefore it has an infimum, which we shall call e_0.

Because e_0 is the infimum, we can take a sequence, u_n, so that the energy on this sequence decreases to e_0.

Next, we show that there is a subsequence of the u_n which converges to a function u weakly (this basically means convergence as a linear functional on H^1). To do this, we know that the H^1-norm on this sequence is bounded above, because we have this inequality with the energy, and we know the energy is bounded. We then apply something called the Banach–Alaoglu theorem, which says that a bounded sequence has a weakly convergent subsequence.

Now we need to show that the energy of u actually is e_0.

On the one hand, e_0 is the infimum over H^1, so certainly the energy of u is not smaller than e_0.

On the other hand, if we show that E is weakly lower-semicontinuous, which means that the energy of the limit is not larger than the limit of the energy, we have that u is not larger than e_0. (This is done using the same types of inequalities as mentioned on the previous slide.) So they must be equal.

Finally, we need to show that u still has total charge Ne, so none has disappeared somewhere while we were taking the limit. This is equivalent to showing that the integral of the square of the difference tends to zero; this is called strong convergence.

There is a theorem called the Rellich–Kondrashov theorem which basically states that if a sequence is bounded in H^1, it has a sequence that converges strongly in L^2, to v, say.

Then we can show that the strong limit v is the same function as the weak limit u using essentially the Cauchy–Schwarz inequality.

So, all of this together means that this limit u minimises E, and it has the right charge, Ne. Therefore it also satisfies the Euler–Lagrange equations, so a solution exists!

Lastly,

I shall discuss some areas to which this result could be extended in future, including more "realistic" systems.

6 Generalisations

- There seems to be a fairly simple extension of the result as just discussed to manifolds with boundary: these people have a result for compact subsets in $\mathbb{R}^3$ with smooth boundary, and the technique can probably be extended to more general manifolds; the only difficulty is probably generalising the consistency conditions.
- Six dimensions is a curious borderline case: there are exact results for similar systems in six dimensions, but the functional I have discussed is not suitable; there may be a slightly different definition which does extend.
- Non-compact manifolds, such as $\mathbb{R}^n$, are harder, mainly due to the tension that arises between showing that the energy is finite, and showing that the charge does not leak away when taking the limit.
- There is no reason the manifold needs to be smooth: it should be sufficient to have a sensible Laplacian on it, for which C^2 is sufficient.

- A number of results of this type are known in three dimensions: in particular, there is this result, which shows that hydrogen atoms are stable, even when the electron can self-interact. The proof uses the same principles, but is considerably more complicated than what I have explained here.
- Finally, for those of you still wondering about the Maxwell–Klein–Gordon system I mentioned at the beginning, the natural setting is a Lorentzian manifold, which we know is much harder to deal with. Also, the Gauss's Law-type equation becomes a Schrödinger-type equation, which cannot be tackled in the same way.

Thank you.