A variational formulation for relativistic mechanics and a new interpretation for the Bohr atomic model

Fabio Silva Botelho
Department of Mathematics
Federal University of Santa Catarina, UFSC
Florianópolis, SC - Brazil

Abstract

This article develops a variational formulation for the relativistic Klein-Gordon equation. The main results are obtained through an extension of the classical mechanics approach to a more general context, which in some sense, includes the quantum mechanics one. For the second part of the text, the definition of normal field and its relation with the wave function concept play a fundamental role in the main results establishment.

1 Introduction

In this work we propose a variational formulation for the Klein-Gordon relativistic equation obtained through an extension of the classical mechanics approach to a more general context.

We introduce a energy part aiming to minimize and control, in a specific appropriate sense to be described in the next sections, the curvature field distribution along the concerned mechanical system.

About the references, this work is based on the book [7] and the articles [4, 5]. Indeed, in the next sections we present some results similar to those presented in [7] and [5]. In the third section we develop in details one of the main results, namely, the establishment of the Klein-Gordon relativistic equation resulted from the respective variational formulation.

At this point we remark that details on the Sobolev Spaces involved may be found in [1, 6]. For standard references in quantum mechanics, we refer to [3, 8, 9] and the non-standard [2].

Finally, we emphasize this article is not about Bohmian mechanics, even though the David Bohm work has been always inspiring.

2 The Newtonian approach

In this section, specifically for a free particle context, we shall obtain a close relationship between classical and quantum mechanics.
Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial \Omega$, on which we define a position field, in a free volume context, denoted by $r : \Omega \times [0, T] \to \mathbb{R}^3$, where $[0, T]$ is a time interval.

Suppose also an associated density distribution scalar field is given by $(\rho \circ r) : \Omega \times [0, T] \to [0, +\infty)$, so that the kinetics energy for such a system, denoted by $J : U \times V \to \mathbb{R}$, is defined as

$$ J(r, \rho) = \frac{1}{2} \int_0^T \int_{\Omega} \rho(r(x, t)) \frac{\partial r(x, t)}{\partial t} \cdot \frac{\partial r(x, t)}{\partial t} \sqrt{g} \, dx \, dt, $$

subject to

$$ \int_{\Omega} \rho(r(x, t)) \sqrt{g} \, dx = m, \text{ on } [0, T], $$

where $m$ is the total system mass, $t$ denotes time and $dx = dx_1 \, dx_2 \, dx_3$.

Here,

$$ U = \{ r \in W^{1,2}(\Omega \times [0, T]) : r(x, 0) = r_0(x) \text{ and } r(x, T) = r_1(x), \text{ in } \Omega \}, $$(1)

and

$$ V = \{ \rho(r) \in L^2([0, T]; W^{1,2}(\Omega)) : r \in U \}. $$

Also

$$ g_k = \frac{\partial r(x, t)}{\partial x_k}, $$

where we assume

$$ \{g_k, k \in \{1, 2, 3\}\} $$
to be a linearly independent set in $\Omega \times [0, T]$,

$$ g_{jk} = g_j \cdot g_k, $$

$$ \{g^{ij}\} = \{g_{ij}\}^{-1}, $$

and

$$ g = \det\{g_{jk}\}. $$

For such a standard Newtonian formulation, the kinetics energy takes into account just the tangential field given by the time derivative

$$ \frac{\partial r(x, t)}{\partial t}. $$

At this point, the idea is to complement such an energy with a new term, denoted by $\hat{R}$, which would consider also the control of curvature distribution along the mechanical system.

So, with such statements in mind, we redefine the concerning energy, denoting it again by $J : U \times V \times V_1 \to \mathbb{R}$, as

$$ J(r, \rho) = -\frac{1}{2} \int_0^T \int_{\Omega} \rho(r(x, t)) \frac{\partial r(x, t)}{\partial t} \cdot \frac{\partial r(x, t)}{\partial t} \sqrt{g} \, dx \, dt \\
+ \gamma \int_0^T \int_{\Omega} \hat{R} \sqrt{g} \, dx \, dt, $$

(2)
subject to
\[
\int_{\Omega} \rho(\mathbf{r}(x,t)) \sqrt{g} \, d\mathbf{x} = m, \text{ on } [0,T],
\]
where
\[
\hat{R} = \sum_{i,j,k,l}^{3} g^{ij} g^{kl} \frac{\partial}{\partial x_i} \left( \sqrt{\frac{\rho(x,t)}{m}} \frac{\partial \mathbf{r}(x,t)}{\partial x_j} \right) \cdot \frac{\partial}{\partial x_k} \left( \sqrt{\frac{\rho(x,t)}{m}} \frac{\partial \mathbf{r}(x,t)}{\partial x_l} \right),
\]
and \( \gamma > 0 \) is a constant to be specified.

Thus, defining a complex function \( \phi \) such that
\[
|\phi| = \sqrt{\frac{\rho}{m}}
\]
and observing that the Christoffel symbols \( \Gamma^s_{ij} \) are such that
\[
\frac{\partial^2 \mathbf{r}(x,t)}{\partial x_i \partial x_j} = \sum_{s=1}^{3} \Gamma^s_{ij} \frac{\partial \mathbf{r}(x,t)}{\partial x_s}, \forall i, j \in \{1, 2, 3\},
\]
we have
\[
\frac{\partial}{\partial x_i} \left( \phi \frac{\partial \mathbf{r}(x,t)}{\partial x_j} \right) = \frac{\partial \phi}{\partial x_i} \frac{\partial \mathbf{r}(x,t)}{\partial x_j} + \phi \frac{\partial^2 \mathbf{r}(x,t)}{\partial x_i \partial x_j},
\]
\[
\frac{\partial}{\partial x_i} \left( \phi^* \frac{\partial \mathbf{r}(x,t)}{\partial x_j} \right) = \frac{\partial \phi^*}{\partial x_i} \frac{\partial \mathbf{r}(x,t)}{\partial x_j} + \phi^* \frac{\partial^2 \mathbf{r}(x,t)}{\partial x_i \partial x_j},
\]
\[
\text{Therefore,}
\]
\[
\left( \frac{\partial}{\partial x_i} \left( \phi \frac{\partial \mathbf{r}(x,t)}{\partial x_j} \right) \right) \cdot \left( \frac{\partial}{\partial x_k} \left( \phi^* \frac{\partial \mathbf{r}(x,t)}{\partial x_l} \right) \right) = \left( \frac{\partial \phi}{\partial x_i} \frac{\partial \mathbf{r}(x,t)}{\partial x_j} + \phi \frac{\partial^2 \mathbf{r}(x,t)}{\partial x_i \partial x_j} \right) \cdot \left( \frac{\partial \phi^*}{\partial x_k} \frac{\partial \mathbf{r}(x,t)}{\partial x_l} + \phi^* \frac{\partial^2 \mathbf{r}(x,t)}{\partial x_k \partial x_l} \right)
\]
\[
= \sum_{s,p=1}^{3} \left( g_{ji} \frac{\partial \phi}{\partial x_i} \frac{\partial \phi^*}{\partial x_k} + \phi \frac{\partial \phi^*}{\partial x_k} \Gamma^s_{ij} g_{sl} + \phi^* \frac{\partial \phi}{\partial x_i} \Gamma^p_{kl} g_{pj} + |\phi|^2 \Gamma^s_{ij} \Gamma^p_{kl} g_{sp} \right).
\]
From this, we may write,
\[
\hat{R} = \sum_{i,j,k,l,p,s=1}^{3} g^{ij} g^{kl} \left( g_{ji} \frac{\partial \phi}{\partial x_i} \frac{\partial \phi^*}{\partial x_k} + \phi \frac{\partial \phi^*}{\partial x_k} \Gamma^s_{ij} g_{sl} + \phi^* \frac{\partial \phi}{\partial x_i} \Gamma^p_{kl} g_{pj} + |\phi|^2 \Gamma^s_{ij} \Gamma^p_{kl} g_{sp} \right).
\]
Already including the Lagrange multipliers concerning the restrictions, the final expression for the energy, denoted by $J : U \times V \to \mathbb{R}$, would be given by

$$J(r, \phi, E) = -\frac{1}{2} \int_0^T \int_\Omega m|\phi(r(x, t))|^2 \left(\frac{\partial r(x, t)}{\partial t}\right) \cdot \left(\frac{\partial r(x, t)}{\partial t}\right) \sqrt{g} \, dx \, dt + \frac{\gamma}{2} \int_0^T \int_\Omega \hat{R} \sqrt{g} \, dx \, dt - m \int_0^T E(t) \left(\int_\Omega |\phi(r)|^2 \sqrt{g} \, dx - 1\right) \, dt,$$

where,

$$U = \{ r \in W^{1,2}(\Omega \times [0, T]) : r(x, 0) = r_0(x) \text{ and } r(x, T) = r_1(x), \text{ in } \Omega \},$$

Finally, in particular for the special case in which $r(x, t) \approx x$,

we get

$$\frac{\partial r(x, t)}{\partial t} \approx 0,$$

$g_k \approx e_k$, where

$$\{e_1, e_2, e_3\}$$

is the canonical basis of $\mathbb{R}^3$.

Therefore, in such a case,

$$\frac{\gamma}{2} \int_0^T \int_\Omega \hat{R} \sqrt{g} \, dx \, dt \approx \frac{\gamma T}{2} \sum_{k=1}^3 \int_\Omega \frac{\partial \phi}{\partial x_k} \frac{\partial \phi^*}{\partial x_k} \, dx.$$

Hence, with such last results we may infer that

$$J(r, \phi, E)/T = \tilde{J}(\phi, E)$$

$$= \frac{\gamma}{2} \sum_{k=1}^3 \int_\Omega \frac{\partial \phi}{\partial x_k} \frac{\partial \phi^*}{\partial x_k} \, dx$$

$$- E \left(\int_\Omega |\phi|^2 dx - 1\right).$$

This last energy is just the standard Schrödinger one in a free particle context.

3 A brief note on the relativistic context, the Klein-Gordon equation

Of particular interest is the case in which $x = (x_1, x_2, x_3) \in \mathbb{R}^3$ and point-wise,

$$r(x, t) = (ct, X_1(t, x), X_2(t, x), X_3(t, x)),$$
where
\[ M = \{ r(x, t) : (x, t) \in \Omega \times [0, T] \}, \]
for an appropriate \( \Omega \subset \mathbb{R}^3 \).

Also, denoting \( dx = dx_1 dx_2 dx_3 \), the mass differential would be given by
\[
dm = \rho(r) \sqrt{1 - \frac{v^2}{c^2}} \sqrt{-g} \, dx = \frac{|R(r)|^2}{\sqrt{1 - \frac{v^2}{c^2}}} \sqrt{-g} \, dx,
\]
and the semi-classical kinetics energy differential would be expressed by
\[
dE_c = \frac{\partial r(t, x)}{\partial t} \cdot \frac{\partial r(t, x)}{\partial t} \, dm
= -\left( \frac{\partial \rho}{\partial t} \right)^2 \, dm
= -(c^2 - v^2) \, dm,
\]
so that
\[
dE_c = -c^2 (\sqrt{1 - \frac{v^2}{c^2}})|R(r)|^2 \sqrt{-g} \, dx,
\]
where
\[
\partial^2 = c^2 dt^2 - dX_1(t, x)^2 - dX_2(t, x)^2 - dX_3(t, x)^2.
\]

Thus, the concerning energy is expressed by,
\[
J_1(r, R) = -\int_0^T \int_{\Omega} dE_c \, dt + \frac{\gamma}{2} \int_0^T \int_{\Omega} \hat{R} \sqrt{-g} \, dx \, dt
= c^2 \int_0^T \int_{\Omega} |R(r)|^2 \sqrt{1 - \frac{v^2}{c^2}} \sqrt{-g} \, dx \, dt
+ \frac{\gamma}{2} \int_0^T \int_{\Omega} \hat{R} \sqrt{-g} \, dx \, dt,
\]
subject to
\[
R(r(x, 0)) = R_0(x)
R(r(x, T)) = R_1(x)
\]
and
\[
R(r(x, t)) = 0, \text{ on } \partial \Omega \times [0, T],
\]
\[
\int_{\Omega} |R(r)|^2 \sqrt{-g} \, dx = m, \text{ on } [0, T].
\]

Here, we have denoted
\[
x_0 = ct,
(x_0, x) = (x_0, x_1, x_2, x_3),
g_k = \frac{\partial r(t, x)}{\partial x_k},
\]
where we assume
\[ \{g_k, \ k \in \{0, 1, 2, 3\}\} \]
to be a linearly independent set in \(\Omega \times [0, T]\),
\[ g = \text{det}\{g_{ij}\}, \]
\[ g_{ij} = g_i \cdot g_j, \]
\[ \{g^{ij}\} = \{g_{ij}\}^{-1}, \]
where such a product is given by
\[ y \cdot z = -y_0 z_0 + \sum_{i=1}^{3} y_i z_i, \quad \forall y = (y_0, y_1, y_2, y_3), \quad z = (z_0, z_1, z_2, z_3) \in \mathbb{R}^4. \]

Moreover,
\[ \hat{R} = \sum_{i,j,k,l=0}^{3} g^{ij} g^{kl} \frac{\partial}{\partial x_i} \left( \frac{R(x, t) \frac{\partial r(x, t)}{\partial x_j}}{\sqrt{m}} \right) \frac{\partial}{\partial x_k} \left( \frac{R(x, t) \frac{\partial r(x, t)}{\partial x_l}}{\sqrt{m}} \right). \]

Therefore, defining \(\phi \in W^{1,2}(\Omega \times [0, T]; \mathbb{C})\) as
\[ \phi(x, t) = \frac{R(r(x, t))}{\sqrt{m}}, \]
and recalling that the Christoffel symbols \(\Gamma^s_{ij}\) are such that
\[ \frac{\partial^2 r(x, t)}{\partial x_i \partial x_j} = \sum_{s=0}^{3} \Gamma^s_{ij} \frac{\partial r(x, t)}{\partial x_s}, \quad \forall i, j \in \{0, 1, 2, 3\}, \]
similarly as in the last section, we may obtain
\[ \hat{R} = \sum_{i,j,k,l,p,s=0}^{3} g^{ij} g^{kl} \left( g_{jl} \frac{\partial \phi}{\partial x_i} \frac{\partial \phi^*}{\partial x_k} + \phi \frac{\partial \phi^*}{\partial x_k} \Gamma^s_{ij} g_{sl} \right. \]
\[ + \phi^* \frac{\partial \phi}{\partial x_i} \Gamma^p_{kl} g_{pj} + \left| \phi \right|^2 \Gamma^s_{ij} \Gamma^p_{kl} g_{sp} \right). \]

Finally, we would also have
\[ v = \sqrt{\left( \frac{\partial X_1}{\partial t} \right)^2 + \left( \frac{\partial X_2}{\partial t} \right)^2 + \left( \frac{\partial X_3}{\partial t} \right)^2}. \]

In particular for the special case in which
\[ r(x, t) \approx (ct, x), \]
so that
\[ \frac{\partial r(x, t)}{\partial t} \approx (c, 0, 0, 0), \]
we would obtain
\[ g_0 \approx (1, 0, 0, 0), \ g_1 \approx (0, 1, 0, 0), \ g_2 \approx (0, 0, 1, 0) \text{ and } g_3 \approx (0, 0, 0, 1) \in \mathbb{R}^4. \]

so that
\[
\frac{\gamma}{2} \int_0^T \int_\Omega \sqrt{g} \, dx \, dt \approx \frac{\gamma}{2} \int_0^T \int_\Omega \left( -\frac{1}{c^2} \frac{\partial \phi(x, t)}{\partial t} \frac{\partial \phi^*(x, t)}{\partial t} + \sum_{k=1}^3 \frac{\partial \phi(x, t)}{\partial x_k} \frac{\partial \phi^*(x, t)}{\partial x_k} \right) \, dx \, dt,
\]

and
\[
c^2 \int_0^T \int_\Omega |R(x)|^2 \sqrt{1-v^2/c^2} \sqrt{g} \, dx \, dt \approx mc^2 \int_0^T \int_\Omega |\phi(x, t)|^2 \, dx \, dt.
\]

Hence, with such last results we may infer that
\[
J_1(r, \phi, E) \approx \frac{\gamma}{2} \left( \int_0^T \int_\Omega -\frac{1}{c^2} \frac{\partial \phi(x, t)}{\partial t} \frac{\partial \phi^*(x, t)}{\partial t} \, dx \, dt + \sum_{k=1}^3 \int_0^T \int_\Omega \frac{\partial \phi(x, t)}{\partial x_k} \frac{\partial \phi^*(x, t)}{\partial x_k} \, dx \, dt \right)
+ mc^2 \int_0^T \int_\Omega |\phi(x, t)|^2 \, dx \, dt
- m \int_0^T E(t) \left( \int_\Omega |\phi(x, t)|^2 \, dx - 1 \right) \, dt.
\]

The Euler Lagrange equations for such an energy are given by
\[
\frac{\gamma}{2} \left( \frac{1}{c^2} \frac{\partial^2 \phi(x, t)}{\partial t^2} - \sum_{k=1}^3 \frac{\partial^2 \phi(x, t)}{\partial x_k^2} \right)
+ mc^2 \phi(x, t) - E_1(t) \phi(x, t) = 0, \text{ in } \Omega,
\]

where,
\[
\phi(x, 0) = \phi_0(x), \text{ in } \Omega, \\
\phi(x, T) = \phi_1(x), \text{ in } \Omega, \\
\phi(x, t) = 0, \text{ on } \partial \Omega \times [0, T]
\]

and \( E_1(t) = mE(t) \).

Equation (14) is the relativistic Klein-Gordon one.

For \( E_1(t) = E_1 \in \mathbb{R} \) (not time dependent), at this point we suggest a solution (and implicitly related time boundary conditions) \( \phi(x, t) = e^{-\frac{iE_1 t}{\hbar}} \phi_2(x) \), where
\[
\phi_2(x) = 0, \text{ on } \partial \Omega.
\]
Therefore, replacing this solution into equation (14), we would obtain
\[
\left(\frac{\gamma}{2} - \frac{E_1^2}{c^2 \hbar^2} \right) \phi_2(x) - \sum_{k=1}^{3} \frac{\partial^2 \phi_2(x)}{\partial x_k^2} + mc^2 \phi_2(x) - E_1 \phi_2(x) e^{-iE_1 t / \hbar} = 0,
\]
in \(\Omega\).

Denoting
\[
E_2 = -\frac{\gamma E_1^2}{2c^2 \hbar^2} + mc^2 - E_1,
\]
the final eigenvalue problem would stand for
\[
-\frac{\gamma}{2} \sum_{k=1}^{3} \frac{\partial^2 \phi_2(x)}{\partial x_k^2} + E_2 \phi_2(x) = 0, \text{ in } \Omega
\]
where \(E_1\) is such that
\[
\int_{\Omega} |\phi_2(x)|^2 \, dx = 1.
\]

Moreover, from (14), such a solution \(\phi(x, t) = e^{-iE_1 t / \hbar} \phi_2(x)\) is also such that
\[
\frac{\gamma}{2} \left( \frac{1}{c^2} \frac{\partial^2 \phi(x, t)}{\partial t^2} - \sum_{k=1}^{3} \frac{\partial^2 \phi(x, t)}{\partial x_k^2} \right)
+ mc^2 \phi(x, t) = i \hbar \frac{\partial \phi(x, t)}{\partial t}, \text{ in } \Omega.
\]
At this point, we recall that in quantum mechanics,
\[
\gamma = \hbar^2 / m.
\]

Finally, we remark this last equation (15) is a kind of relativistic Schrödinger-Klein-Gordon equation.

4 A new interpretation of the Bohr atomic model

This section develops a new interpretation of Bohr atomic model through classical and quantum mechanics.

In a second step, we consider as a generalization of such a model, the issue of an interacting system comprised by a large amount of same type atoms.

At this point we start to describe such a model.

Let \(\Omega = B_{R_0}(0) \subset \mathbb{R}^3\) be an open ball with center at \(0 \in \mathbb{R}^3\). Let \([0, T]\) be a time interval. For \(n \in \mathbb{N}\), consider a system with \(\sum_{l=0}^{n-1}(2l + 1)\) electrons and the same number of protons, where the protons are supposed to be at rest at \(x = 0 \in \mathbb{R}^3\). Moreover, the electrons are distributed in \(n\) layers \(l \in \{0, \ldots, n - 1\}\), each layer \(l\) with \(2l + 1\) electrons.

We denote the position field for the electron \(j \in -l, \ldots, 0, \ldots, l\) at the layer \(l\), by \(r_j^l : \Omega \times [0, T] \to \mathbb{R}^3\), where
\[
\begin{align*}
  r_j^l(x, t) &= R_j^l(r) \left( \sin((w_1)_j^l(x)t + \theta_j^l) \cos((w_2)_j^l(x)t + \phi_j^l)i 
                   + \sin((w_1)_j^l(x)t + \theta_j^l) \sin((w_2)_j^l(x)t + \phi_j^l)j + \cos((w_1)_j^l(x)t + \theta_j^l)k \right). \quad (16)
\end{align*}
\]
We also recall that $x \in \mathbb{R}^3$ in spherical coordinates corresponds to $(r, \theta, \phi)$ and $\{i, j, k\}$ is the canonical basis of $\mathbb{R}^3$.

Moreover, the density scalar field for such a same electron is denoted by $m_e |\varphi_j^l| \Omega \rightarrow \mathbb{R}$, where

$$\varphi_j^l(x) = \varphi_j(r)(L^{-j})^l (\sin \theta e^{i \phi}),$$

$i$ denotes the imaginary unit,

$$L_x = -\hbar \left( \sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right),$$

$$L_y = \hbar \left( \cos \phi \frac{\partial}{\partial \theta} - \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right)$$

and

$$L^{-} = \frac{1}{\hbar}(L_x - iL_y),$$

and where $(L^{-})^0 = I_d$ (identity operator).

**Remark 4.1.** In principle, we would expect $r_j^l$ to be an injective function, so that

$$\tilde{\varphi}_j^l(r_j^l(x, t)) = \varphi_j(x, t) = \varphi_j((r_j^l(x, t))^{-1})$$

is well defined.

This may not be the case for the motion indicated in (16). Thus, such a concerning motion suggests us a new interpretation of the Bohr atomic model and related wave particle duality for the electrons in the atom in question.

We also define,

$$U = \{\varphi = \{\varphi_j^l\} \in W^{1,2}(\Omega; \mathbb{C}^Z) : \varphi_j^l = 0 \text{ on } \partial\Omega\},$$

and

$$V = \{r = \{r_j^l\} \in W^{1,2}(\Omega \times [0, T]; \mathbb{R}^3) : R_j^l(0) = 0, \text{ and } R_j^l(0) = R_0\}. $$

For such a system, we consider the following types of energy.

1. Kinetics energy, denoted by $E_c$, where

$$E_c = \frac{1}{2} \sum_{l=0}^{n-1} \sum_{j=-l}^{l} \int_0^T \int_\Omega m_e |\varphi_j^l(x)|^2 \frac{\partial r_j^l(x, t)}{\partial t} \cdot \frac{\partial r_j^l(x, t)}{\partial t} \, dx \, dt,$$

where $m_e$ denotes the mass of a single electron and

$$dx = dx_1 dx_2 dx_3.$$

2. A regularizing part for the position field, denoted by $E_r$, where

$$E_r = \frac{1}{2} \sum_{l=0}^{n-1} \sum_{j=-l}^{l} \sum_{k=1}^{3} \int_0^T \int_\Omega A^l |\varphi_j^l(x)|^2 \frac{\partial r_j^l(x, t)}{\partial x_k} \cdot \frac{\partial r_j^l(x, t)}{\partial x_k} \, dx \, dt,$$

with $A^l > 0$ to be specified, $\forall l \in \{0, \ldots, n-1\}$. 9
3. Coulomb electronic interaction (classical), denoted by \( E_{int} \), where in a first approximation, we consider only the interaction for the same layer electrons, neglecting the interactions between different layer electrons.

Thus,

\[
E_{int} = \frac{1}{4} \sum_{l=0}^{n-1} \sum_{j=-l}^{l} \sum_{k=-l}^{l} Ke^2 \int_0^T \int_\Omega \frac{|\varphi_j^l(x)|^2 |\varphi_k^l(x)|^2}{|r_j^l(x, t) - r_k^l(x, t)|} \, dx \, dt,
\]

where \( e \) is the charge of a single electron and \( K > 0 \) is an appropriate constant to be specified.

4. Coulomb interaction of each electron with the heavier nucleus, denoted by \( E_{int}^p \), where

\[
E_{int}^p = \frac{1}{2} \sum_{l=0}^{n-1} \sum_{j=-l}^{l} K e^2 Z \int_0^T \int_\Omega \frac{|\varphi_j^l(x)|^2}{|r_j^l(x, t)|} \, dx \, dt.
\]

5. Energy related to the presence of external potentials \( V_j^l \), denoted by \( E_p \), where

\[
E_p = \frac{1}{2} \sum_{l=0}^{n-1} \sum_{j=-l}^{l} \int_0^T \int_\Omega V_j^l(x)|\varphi_j^l(x)|^2 \, dx \, dt.
\]

6. A regularizing and curvature distribution control term for the scalar density field (quantum part), denoted by \( E_q \), where

\[
E_q = \frac{1}{2} \sum_{l=0}^{n-1} \sum_{j=-l}^{l} \sum_{k=-l}^{l} \gamma_j^l \int_0^T \int_\Omega \frac{\partial(\varphi_j^l(x) \mathbf{n}_j^l(x, t))}{\partial x_k} \cdot \frac{\partial(\varphi_j^l(x) \mathbf{n}_j^l(x, t))}{\partial x_k} \, dx \, dt,
\]

where the normal field \( \mathbf{n}_j^l \) may be given by

\[
\mathbf{n}_j^l(x, t) = \sin((w_1)_j^l(x)t + \theta_j^l) \cos((w_2)_j^l(x)t + \phi_j^l)i + \sin((w_1)_j^l(x)t + \theta_j^l) \sin((w_2)_j^l(x)t + \phi_j^l)j + \cos((w_1)_j^l(x)t + \theta_j^l)k, \quad (17)
\]

so that,

\[
\mathbf{n}_j^l(x, t) \cdot \frac{\partial r_j^l(x, t)}{\partial t} = 0, \text{ in } \Omega \times [0, T],
\]

\( \forall j \in \{-l, \ldots, 0, \ldots, l\}, \forall l \in \{0, \ldots, n-1\} \).

7. Constraints: The system is subject to the following constraints,

\[
\int_\Omega |\varphi_j^l(x)|^2 \, dx = 1, \forall l \in \{0, \ldots, n-1\}, j \in \{-l, \ldots, 0, \ldots, l\}.
\]

Hence, the total system energy is given by the functional \( J : U \times V \times \mathbb{R}^Z \to \mathbb{R} \) where already including the Lagrange multipliers, we have

\[
J(\varphi, r, E) = -E_c + E_r + E_{int} - E_{int}^p + E_p + E_q
- \frac{1}{2} \sum_{l=0}^{n-1} \sum_{j=-l}^{l} E_j^l T \left( \int_\Omega |\varphi_j^l(x)|^2 \, dx - 1 \right). \quad (18)
\]
Summarizing,

\[ J(\varphi, r, E) = \frac{1}{2} \sum_{l=-l}^{l} \int_{0}^{T} \int_{\Omega} m_{e} |\phi_{j}^{l}(x)|^{2} \frac{\partial r_{j}^{l}(x, t)}{\partial t} \cdot \frac{\partial r_{j}^{l}(x, t)}{\partial t} \, dx \, dt \]

\[ + \frac{1}{2} \sum_{l=-l}^{l} \int_{0}^{T} \int_{\Omega} A_{j}^{l} |\phi_{j}^{l}(x)|^{2} \frac{\partial r_{j}^{l}(x, t)}{\partial x_{k}} \cdot \frac{\partial r_{j}^{l}(x, t)}{\partial x_{k}} \, dx \, dt \]

\[ + \frac{1}{4} \sum_{l=-l}^{l} K e^{2} \int_{0}^{T} \int_{\Omega} |\phi_{j}^{l}(x)|^{2} |\phi_{k}^{l}(\tilde{x})|^{2} |r_{j}^{l}(x, t) - r_{k}^{l}(\tilde{x}, t)| \, dxd\tilde{x} dt \]

\[ - \frac{1}{2} \sum_{l=-l}^{l} K e^{2} Z \int_{0}^{T} \int_{\Omega} |\phi_{j}^{l}(x)|^{2} \, dx \, dt \]

\[ + \frac{1}{2} \sum_{l=-l}^{l} \sum_{k=-l}^{k} |\gamma_{j}^{l}(x)|^{2} \int_{0}^{T} \int_{\Omega} \frac{\partial(\phi_{j}^{l}(x)n_{j}^{l}(x, t))}{\partial x_{k}} \cdot \frac{\partial(\phi_{j}^{l}(x)n_{j}^{l}(x, t))}{\partial x_{k}} \, dx \, dt \]

\[ - \frac{1}{2} \sum_{l=-l}^{l} E_{j}^{l} T \left( \int_{\Omega} |\phi_{j}^{l}(x)|^{2} \, dx - 1 \right). \tag{19} \]

With such statements and definitions in mind, we define the control problem of finding \( \{\theta_{j}^{l}, \phi_{j}^{l}\} \in \mathbb{R}^{Z} \times \mathbb{R}^{Z} \), which minimizes

\[ J_{1}(\varphi, r, E) \]

where

\[ J_{1}(\varphi, r, E) \]

\[ = \frac{1}{4} \sum_{l=-l}^{l} \sum_{k=-k}^{k} K e^{2} \int_{0}^{T} \int_{\Omega} |\phi_{j}^{l}(x)|^{2} |\phi_{k}^{l}(\tilde{x})|^{2} \, dx \, dt \]

subject to

1. \( m_{e} |\phi_{j}^{l}(x)|^{2} \frac{\partial^{2} r_{j}^{l}(x, t)}{\partial t^{2}} \)

\[- A_{j}^{l} \sum_{k=1}^{3} \frac{\partial}{\partial x_{k}} \left( |\phi_{j}^{l}(x)|^{2} \frac{\partial r_{j}^{l}(x, t)}{\partial x_{k}} \right) \]

\[- \sum_{k=-l}^{l} |\phi_{j}^{l}(x)|^{2} \int_{\Omega} K e^{2} |\phi_{k}^{l}(\tilde{x})|^{2} (r_{j}^{l}(x, t) - r_{k}^{l}(\tilde{x}, t)) \, \frac{d\tilde{x}}{|r_{j}^{l}(x, t) - r_{k}^{l}(\tilde{x}, t)|^{3}} \]

\[+ K Z e^{2} \frac{\phi_{j}^{l}(x)|^{2}}{|r_{j}^{l}(x, t)|^{3}} r_{j}^{l}(x, t) \]

\[= 0, \text{ in } \Omega \times [0, T], \tag{21} \]

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\[ -m_e \hat{\varphi}_j^l(r) \frac{1}{T} \int_0^T \frac{\partial r_j^l(x, t)}{\partial t} \cdot \frac{\partial r_j^l(x, t)}{\partial t} \, dt + \]
\[ -\gamma_j^l \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \hat{\varphi}_j^l(r)}{\partial r} \right) \]
\[ + \gamma_j^l \frac{l(l+1)}{r^2} \hat{\varphi}_j^l(r) \]
\[ + \gamma_j^l \hat{\varphi}_j^l(r) \frac{1}{T} \int_0^T \sum_{k=1}^3 \left( \frac{\partial n_j^l}{\partial x_k} \cdot \frac{\partial n_j^l}{\partial x_k} \right) \, dt \]
\[ + \sum_{k=-l}^l \hat{\varphi}_j^l(r) \frac{1}{T} \int_0^T \int_{\Omega} \frac{K e^2 |\varphi_k^l(\tilde{x})|^2}{|r_j^l(x, t) - r_k^l(\tilde{x}, t)|} \, d\tilde{x} dt \]
\[ -KZe^2 \hat{\varphi}_j^l(r) \]
\[ -E_j^l \hat{\varphi}_j^l(r) = 0, \text{ in } [0, R_0], \] (22)

and up to a normalizing constant for \( \varphi(x) \),

\[ \int_0^{R_0} |\hat{\varphi}_j^l(r)|^2 r^2 \, dr = 1, \]

\( \forall j \in \{-l, \ldots, 0, \ldots, l\}, \forall l \in \{0, \ldots, n-1\} \).

5 A system with a large number of interacting atoms

Now consider a system with a large number \( N \) of interacting same type atoms, each one with \( Z = \sum_{l=0}^{n-1} (2l+1) \) electrons and the same number of protons.

Consider also the problem of finding the \( N \) nucleus positions, each one comprised by \( Z \) protons, in an open, bounded, connected set \( \Omega \subset \mathbb{R}^3 \) with a Lipschitzian boundary denoted by \( \partial \Omega \).

We define the position field for the electron \( j \), in the layer \( l \) at the atom \( k \), which the nucleus is located at \( x_k \in \Omega \), denoted by \( r_j^l(\cdot, x_k, \cdot) : \Omega \times [0, T] \to \mathbb{R}^3 \), as

\[ r_j^l(x, x_k, t) = x_k + R_j^l(x, x_k) e^{i\omega_j^l(x, x_k) t} \] (23)

Also, the respective density scalar field is denoted by \( \varphi = \{ \varphi_j^l : \Omega \to \mathbb{C} \} \).

Here

\( \varphi(\cdot, x_k) \in U, \forall k \in \{1, \ldots, N\} \)

and

\( \varphi(\cdot, x_k) \in V, \forall k \in \{1, \ldots, N\} \).
With such statements in mind, we consider the control problem of finding \( \{x_k\}_{k=1}^N \) and \( \{w_j(x, x_k)\} \) which minimizes \( J_2 + J_3 + J_4 \), where

\[
J_2 = \sum_{l_1=0}^{n-1} \sum_{l_2=0}^{n-1} \sum_{l_1}^{t_2} \sum_{l_1 = -l_2}^{k=1} \sum_{l_2=1}^{N} \sum_{l_2=1}^{N} K e^2 \times
\int_0^T \int_\Omega \int_\Omega \frac{|\varphi_j^1(x, x_{k_1})|^2|\varphi_j^2(\bar{x}, x_{k_2})|^2}{|J_j^1(x, x_{k_1}, t) - J_j^2(\bar{x}, x_{k_2}, t)|} \ dx \ dx \ dx dt
\]

(24)

\[
J_3 = \sum_{l=0}^{n-1} \sum_{j=-l}^{N} \sum_{k=1}^{N} \sum_{k=1}^{N} Ke^2 Z \int_0^T \int_\Omega \frac{|\varphi_j^1(x, x_k)|^2}{|J_j^1(x, x_k, t) - x_{k_1}|} \ d x dt,
\]

(25)

and

\[
J_4 = \sum_{k=1}^{N} \sum_{k=1}^{N} Ke^2 Z^2 \frac{1}{|x_k - x_{k_1}|}
\]

subject to

1.

\[
m_e |\varphi_j^1(x, x_k)|^2 \frac{\partial^2 J_j^1(x, x_k, t)}{\partial t^2} - \sum_{s=1}^3 A_i \frac{\partial}{\partial x_s} \left( |\varphi_j(x, x_k)|^2 \frac{\partial J_j^1(x, x_k, t)}{\partial x_s} \right)
\]

\[
- \sum_{l_1=0}^{n-1} \sum_{l_2=0}^{n-1} \sum_{l_1 = -l_2}^{k=1} \sum_{l_2=1}^{N} Ke^2 |\varphi_j^1(x, x_k)|^2 \int_\Omega \frac{|\varphi_j^1(\bar{x}, x_{k_1})|^2 (J_j^1(x, x_k, t) - J_j^1(\bar{x}, x_{k_1}, t))}{|J_j^1(x, x_k, t) - J_j^1(\bar{x}, x_{k_1}, t)|^3} \ d \bar{x}
\]

\[
+ Ke^2 Z \sum_{k=1}^{N} \frac{|\varphi_j^1(x, x_k)|^2 (J_j^1(x, x_k, t) - x_{k_1})}{|J_j^1(x, x_k, t) - x_{k_1}|^3}
\]

\[
= 0, \text{ in } \Omega.
\]

(26)

2.

\[
n_j^1(x, x_k, t) \cdot \frac{\partial^2 J_j^1(x, x_k, t)}{\partial t} = 0, \text{ in } \Omega \times [0, T],
\]

3.

\[
n_j^1(x, x_k, t) \cdot n_j^1(x, x_k, t) = 1, \text{ in } \Omega \times [0, T],
\]
4.

\[- \sum_{s=1}^{3} \gamma^s \frac{\partial^2 \varphi^l_j(x, x_k)}{\partial x^2_s} \]

\[+ \frac{1}{T} \sum_{s=1}^{3} \left( \frac{\partial m^l_j(x, x_k, t)}{\partial x^s} \cdot \frac{\partial m^l_j(x, x_k, t)}{\partial x^s} \right) dt \]

\[+ \varphi^l_j(x, x_k) \int_0^T \sum_{l=0}^{n-1} \sum_{k=-1}^{l_1} \sum_{k_1=1}^{N} \frac{1}{T} \int_{\Omega} |r^l_j(x, x_k) - r^l_i(\tilde{x}, x_k)|^2 d\tilde{x}dt \]

\[- \sum_{s=1}^{3} A^l \varphi^l_j(x, x_k) \frac{1}{T} \int_0^T \frac{\partial r^l_j(x, x_k, t)}{\partial x^s} \cdot \frac{\partial r^l_j(x, x_k, t)}{\partial x^s} dt \]

\[- m_c \varphi^l_j(x, x_k) \frac{1}{T} \int_0^T \frac{\partial r^l_j(x, x_k, t)}{\partial t} \cdot \frac{\partial r^l_j(x, x_k, t)}{\partial t} dt \]

\[- E^l_{jk} \varphi^l_j(x, x_k) = 0, \text{ in } \Omega. \] (27)

5.

\[\int_{\Omega} |\varphi^l_j(x, x_k)|^2 dx = 1, \forall l \in \{0, \ldots, n-1\}, j \in \{-l, \ldots, 0, \ldots, l\}, k \in \{1, \ldots, N\}.\]

5.1 A proposal for the case in which \(N\) is very large

As \(N\) is very large, we shall propose a limit density scalar field \(\varphi^l_j(x, y)\), that is

\[\varphi^l_j : \Omega \times \Omega \rightarrow \mathbb{C}.\]

Also, we shall propose, as the position vector field, \(r^l_j(x, y, t)\), that is \(r^l_j : \Omega \times \Omega \times [0, T] \rightarrow \mathbb{R}^3\), where

\[r^l_j(x, y, t) = y + R^l_j(x, y) e^{iw^l_j(x, y)t}.\] (28)

We assume \(\varphi = \{\varphi^l_j\} \in U\), where

\[U = \{\varphi = \{\varphi^l_j\} \in W^{1,2}(\Omega \times \Omega; \mathbb{C}^2) : \varphi^l_j = 0 \text{ on } \partial \Omega\}\]

and \(r = r^l_j \in V\), where here

\[V = \{r = r^l_j \in W^{1,2}(\Omega \times \Omega \times [0, T]; \mathbb{R}^3) : R^l_j = 0 \text{ on } \partial(\Omega \times \Omega)\}.\]

For the protons, we specify the density scalar field \(\varphi_p : \Omega \times \Omega \rightarrow \mathbb{C}\), and the respective position field \(r^l_p(x, y) = y\). Moreover, \(\varphi_p \in U_p\), where

\[U_p = \{\varphi_p \in W^{1,2}(\Omega \times \Omega; \mathbb{C}) : \varphi_p(x, y) = 0, \text{ in } \partial(\Omega \times \Omega)\}.\]
In the distributional sense, we should approximately expect to obtain

$$\varphi_p(x, y) = \delta(x - y), \text{ in } (\Omega \times \Omega)^0$$

where \((\Omega \times \Omega)^0\) denotes the interior of \(\Omega \times \Omega\). Also, \(\delta(x - y)\) denotes a standard Dirac delta.

With such statements in mind, we consider the control problem of finding \(\{w^j\}\) which minimizes \(J_2 + J_3 + J_4\), where

\[
J_2 = \sum_{l=0}^{n-1} \sum_{j=-l}^{l_1} K e^2 \times \int_0^T \int_0^T \int_0^T \int_0^T \int_0^T \frac{|\varphi_j^l(x, y)|^2 |\varphi_j^l(\tilde{x}, \tilde{y})|^2}{|r_j^l(x, y, t) - r_j^l(\tilde{x}, \tilde{y}, t)|} \, dx \, d\tilde{x} \, dy \, d\tilde{y} \, dt 
\]

\[
J_3 = \sum_{l=0}^{n-1} \sum_{j=-l}^{l_1} K e^2 Z \int_0^T \int_0^T \int_0^T \int_0^T \int_0^T \frac{|\varphi_j^l(x, y)|^2}{|r_j^l(x, y, t) - \tilde{y}|} \, dx \, dy \, d\tilde{y} \, dt, \tag{29}
\]

and

\[
J_4 = T \int_\Omega \int_\Omega \int_\Omega \int_\Omega \frac{K e^2 Z^2 |\varphi_p(x, y)|^2 |\varphi_p(\tilde{x}, \tilde{y})|^2}{|y - \tilde{y}|} \, dx \, d\tilde{x} \, dy \, d\tilde{y},
\]

subject to

1. \[m |\varphi_j^l(x, y)|^2 \frac{\partial^2 r_j^l(x, y, t)}{\partial t^2} - A^l \sum_{s=1}^3 \left( \frac{\partial}{\partial x_s} \left( |\varphi(x, y)|^2 \frac{\partial r_j^l(x, y, t)}{\partial x_s} \right) \right) + \frac{\partial}{\partial y_s} \left( |\varphi(x, y)|^2 \frac{\partial r_j^l(x, y, t)}{\partial y_s} \right) \]

\[- n \sum_{l=0}^{n-1} \int_0^T \int_0^T \int_\Omega \frac{|\varphi_j^l(x, y)|^2}{|r_j^l(x, y, t) - r_j^l(\tilde{x}, \tilde{y}, t)|^3} \, dx \, d\tilde{x} \, dy \]

\[+ K e^2 Z |\varphi_j^l(x, y)|^2 \int_0^T \int_0^T \int_\Omega \frac{|r_j^l(x, y, t) - \tilde{y}|}{|r_j^l(x, y, t) - \tilde{y}|^3} \, d\tilde{y} \]

\[= 0, \text{ in } \Omega \times \Omega \times [0, T]. \tag{31}\]

2. \[n_j^l(x, y, t) \cdot \frac{\partial r_j^l(x, y, t)}{\partial t} = 0, \text{ in } \Omega \times \Omega \times [0, T], \]

3. \[n_j^l(x, y, t) \cdot n_j^l(x, y, t) = 1, \text{ in } \Omega \times \Omega \times [0, T], \]
4. 
\[-\gamma_j^l \sum_{s=1}^3 \left( \frac{\partial^2 \varphi_j^l(x, y)}{\partial x_s^2} + \frac{\partial^2 \varphi_j^l(x, y)}{\partial y_s^2} \right) \]
\[+ \gamma_j^l \varphi_j^l(x, y) \frac{1}{T} \int_0^T \sum_{s=1}^3 \left( \left( \frac{\partial n_j^l(x, y, t)}{\partial x_s} \cdot \frac{\partial n_j^l(x, y, t)}{\partial x_s} \right) + \left( \frac{\partial n_j^l(x, y, t)}{\partial y_s} \cdot \frac{\partial n_j^l(x, y, t)}{\partial y_s} \right) \right) dt \]
\[+ \varphi_j^l(x, y) \sum_{l_1=0}^{n-1} \sum_{k=-l_1}^{l_1} \frac{1}{T} \int_0^T \int_\Omega \int_\Omega \frac{|\varphi_k^l(\tilde{x}, \tilde{y})|^2}{|r_j^l(x, y, t) - r_k^l(\tilde{x}, \tilde{y}, t)|} d\tilde{x}d\tilde{y} dt \]
\[- K e^2 Z \varphi_j^l(x, y) \int_\Omega \int_\Omega \frac{|\varphi_j^l(x, y)|^2}{|r_j^l(x, y, t) - y|^2} d\tilde{x}d\tilde{y} dt \]
\[-m_e \varphi_j^l(x, y) \frac{1}{T} \int_0^T \frac{\partial n_j^l(x, y, t)}{\partial t} \cdot \frac{\partial n_j^l(x, y, t)}{\partial t} dt \]
\[-E_j^l(y) \varphi_j^l(x, y) = 0, \text{ in } \Omega \times \Omega, \quad (32) \]

5. 
\[\int_\Omega |\varphi_j^l(x, y)|^2 dx = 1, \quad \forall l \in \{0, \ldots, n-1\}, \quad j \in \{-l, \ldots, 0, \ldots, l\}, \quad y \in \Omega, \]

6. 
\[-\gamma_p \sum_{s=1}^3 \left( \frac{\partial^2 \varphi_p(x, y)}{\partial x_s^2} + \frac{\partial^2 \varphi_p(x, y)}{\partial y_s^2} \right) \]
\[+ \varphi_p(x, y) \sum_{l=0}^{n-1} \frac{K e^2 Z}{T} \int_0^T \int_\Omega \int_\Omega \frac{|\varphi_j^l(\tilde{x}, \tilde{y})|^2}{|\tilde{y} - r_j^l(\tilde{x}, \tilde{y}, t)|} d\tilde{x}d\tilde{y} dt \]
\[-K e^2 Z^2 \varphi_p(x, y) \int_\Omega \int_\Omega \frac{|\varphi_j^l(\tilde{x}, \tilde{y})|^2}{|\tilde{y} - y|^2} d\tilde{x}d\tilde{y} \]
\[-E_p(y) \varphi_p(x, y) = 0, \text{ in } \Omega \times \Omega. \quad (33) \]

7. 
\[\int_\Omega |\varphi_p(x, y)|^2 dx = 1, \quad \forall y \in \Omega. \]

6 Conclusion

In this article we have developed a variational formulation for the relativistic Klein-Gordon equation by extending the standard classical mechanics energy to a more general functional.
We believe the results here presented may be applied and extended to other models in mechanics, including the quantum and relativistic approaches for the study of atoms and molecules. Finally, we have the objective and interest in applying such results also for the case in which electromagnetic fields are included, however we postpone such developments for a future research.

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