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Derivation of classical and quantum mechanical effects for charged particles from dynamics of PDE

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Classical Electromagnetic Theory. Point Charge in EM Field

Newton's law for point of mass m :

$$\frac{d}{dt}\left[m\frac{d}{dt}\mathbf{r}\left(t\right)\right]=f\left(t,\mathbf{r}\right),$$

Lorentz force for charge q in EM field:

$$f\left(t,\mathbf{r}\right)=q\left[\mathbf{E}\left(t,\mathbf{r}\left(t\right)\right)+\frac{1}{c}\mathbf{v}\left(t\right)\times\mathbf{B}\left(t,\mathbf{r}\left(t\right)\right)\right],\qquad \mathbf{v}=\frac{d}{dt}\mathbf{r}$$

where $\mathbf{E}$ and $\mathbf{B}$ are the electric field and the magnetic induction.

EM field generated by a moving point charge:

$$\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t}+\nabla\times\mathbf{E}=\mathbf{0},\qquad \nabla\cdot\mathbf{B}=0,$$

$$\begin{aligned}\frac{1}{c}\frac{\partial\mathbf{E}}{\partial t}-\nabla\times\mathbf{B} &= -\frac{4\pi}{c}q\delta\left(\mathbf{x}-\mathbf{r}\left(t\right)\right)\mathbf{v}\left(t\right),\\ \nabla\cdot\mathbf{E} &= 4\pi q\delta\left(\mathbf{x}-\mathbf{r}\left(t\right)\right),\end{aligned}$$

Electromagnetic potentials $\varphi,\mathbf{A}$

$$\mathbf{E}=-\nabla\varphi-\frac{1}{c}\partial_t\mathbf{A},\qquad \mathbf{B}=\nabla\times\mathbf{A}.$$

Inherent Difficulties

Singularities and divergencies. Coulomb's potential for $\mathbf{r} = const$

$$\nabla^2 \varphi = -4\pi q \delta(\mathbf{x} - \mathbf{r}), \qquad \varphi = \frac{q}{|\mathbf{x} - \mathbf{r}|}$$

Singularity at $\mathbf{x} = \mathbf{r}$ (exactly at location of the charge)
Abraham model: replace $\delta(\mathbf{x} - \mathbf{r})$ by a regularized function $\tilde{\delta}_a(\mathbf{x} - \mathbf{r})$,

$$\tilde{\delta}_a(\mathbf{x}) \to \delta(\mathbf{x}) \text{ as } \quad a \to 0$$

$\tilde{\delta}_a$ is proportional to characteristic function of a ball or a sphere with radius a .

$$\int \tilde{\delta}_a(\mathbf{x})\, dx = 1$$

Preserve Newton's equations for the center with Lorentz force. Poincare: cohesion forces should be taken into account (Poincare stresses).

Problems remain at atomic scales: classical treatment of Rutherford model of atom does not produce *discrete energy levels* .
Non-classical solution:
Bohr model; Schrodinger model

Neoclassical model for electric charges

Babin A. and Figotin A., Wave-Corpuscle Mechanics for Electric Charges, Journal of Statistical Physics, v. 138, pp. 912–954, 2010.

Babin A. and Figotin A., Some mathematical problems in a neoclassical theory of electric charges, Dicrete and Continuous Dynamical Systems, **27**, 4, pp. 1283-1326, 2010.

Babin A. and Figotin A., Electrodynamics of balanced charges, Foundations of Physics, 2010, available on-line.

versions with more details available in Archiv

Our requirements for a model: *One theory for macroscopic and atomic spatial scales*

(i) Dynamical equations for multiple charges coupled with EM fields can be derived from a relativistic invariant Lagrangian

(ii) Non-relativistic (small velocities) case can be derived from relativistic as $\frac{v}{c} \to 0$

(iii) Newton's law with Lorentz force is not imposed but has to be derived for macroscopic scales of order R from field equations as $a/R \to 0$

(iv) Hydrogen atom can be described by a system for two opposite charges (the size of a cannot be neglected). Solutions should have discrete energy levels as in Bohr and Schrodinger models.

Differences with classical models (Abraham, Kiessling, Spohn, Komech, Lorentz, ...):

A charge is not a point but is described by a scalar *function* $\psi^{\ell}(t, \mathbf{x})$

Shape of charge distribution $\psi^{\ell}(t, \mathbf{x})$ for $\ell-$th charge *is not prescribed* as in Abraham model but is found from equations as well as law of motion

Relativistic case: Dynamics of ψ^{ℓ} is determined by Nonlinear Klein-Gordon equation (NLKG) for ψ^{ℓ} coupled with Maxwell equations

Non-relativistic case: Dynamics of ψ^{ℓ} is determined by Nonlinear Schrodinger equation (NLS) for ψ^{ℓ} coupled with reduced Maxwell equations where terms with $\frac{1}{c}$ are neglected

Non-relativistic theory

Nonlinear Schrodinger equation (NLS)

$$i\hbar\partial_t\psi^\ell = -\frac{\hbar^2}{2m^\ell}\left(\tilde{\nabla}_{ex}^\ell\right)^2\psi^\ell + q^\ell\left(\varphi_{\neq\ell}+\varphi_{ex}\right)\psi^\ell + \frac{\hbar^2}{2m^\ell}\left[G_a^\ell\right]'\left(\left|\psi^\ell\right|^2\right)\psi^\ell,$$

with electric potential φ^ℓ

$$\nabla^2\varphi^\ell = -4\pi q^\ell\left|\psi^\ell\right|^2, \ell = 1, ..., N.$$

$$\varphi_{\neq\ell} = \sum_{\ell'\neq\ell}\varphi^{\ell'}, \tilde{\nabla}_{ex}^\ell = \nabla - \frac{iq^\ell\mathbf{A}_{ex}}{\hbar c}$$

$\varphi_{ex}, \mathbf{A}_{ex}$ are potentials of external fields, $\hbar > 0$ is Planck constant $\hbar = \frac{h}{2\pi}$ and $\left[G_a^\ell\right]'$ is the nonlinearity.

$$G_a'(s) = a^{-2}G_1'\left(a^3 s\right)$$

a is size parameter, $a << R$ where R is macroscopic scale of variation $\varphi_{ex}, \mathbf{A}_{ex}$

General properties

General property of NLS: for any regular solution $\partial_t \left\|\psi^\ell\right\|^2 = 0$ (charge conservation). We impose normalization condition

$$\left\|\psi^\ell\right\|^2 = \int \left|\psi^\ell\right|^2 dx = 1$$

(ensures Coulomb normalization of potential). Nonlinearity depends on size parameter parameter a

$$G_a'(s) = a^{-2} G_1'\left(a^3 s\right)$$

Nonlinearity is chosen so that NLS when external fields vanish has an equilibrium (ground state)

$$0 = -\frac{\hbar^2}{2m^\ell} \nabla^2 \psi^\ell + \frac{\hbar^2}{2m^\ell} \left[G_a^\ell\right]' \left(\left|\psi^\ell\right|^2\right) \psi^\ell$$

which depends on size parameter a

$$\mathring{\psi}(r) = \mathring{\psi}_a(r) = a^{-3/2} \mathring{\psi}_1\left(a^{-1} r\right),$$

$$\int \left|\mathring{\psi}_a\right|^2 dx = 1$$

Obviously

$$\left|\mathring{\psi}_a\right|^2 \to \delta(x) \quad \text{as} \quad a \to 0$$

Nonlinearity

Do such nonlinearities exist? Consider a given ground state with size parameter a

$$\mathring{\psi}(r) = \mathring{\psi}_a(r) = a^{-3/2}\mathring{\psi}_1\left(a^{-1}r\right),$$

The function $\mathring{\psi}_a(r)$ is assumed to be a smooth positive monotonically decreasing function of $r \geq 0$. The charge equilibrium

$$\nabla^2\mathring{\psi}_a = G_a'\left(\mathring{\psi}_a^2\right)\mathring{\psi}_a.$$

defines the nonlinearity

$$G_1'(s) = \frac{\nabla^2\mathring{\psi}_1(r(s))}{\mathring{\psi}_1(r(s))},\ 0 = \mathring{\psi}_1^2(\infty) \leq s \leq \mathring{\psi}_1^2(0).$$

Example 1. Power law: $\mathring{\psi}_1(r) = c_{pw}\left(1+r^2\right)^{-p}$, $p > 3/4$. Then $G'(s)$ is a linear combination of power laws.

Example 2. Exponentially decaying $\mathring{\psi}_1(r) = c_e e^{-\left(r^2+1\right)^{1/2}}$. For $s \leq c_e^2 e^{-2}$

$$G_1'(s) = 1 - 4/\ln\left(c_e^2/s\right) - 4/\ln^2\left(c_e^2/s\right) - 8/\ln^3\left(c_e^2/s\right).$$

Example 3. *Gaussian form factor* $\mathring{\psi}_1(r) = C_g e^{-r^2/2}$ with $C_g = \pi^{-3/4}$. Such a function is called *gausson* by Bialynicki-Birula and Mycielski. The corresponding *logarithmic nonlinearity*

$$G_a'\left(|\psi|^2\right) = -a^{-2}\ln\left(a^3|\psi|^2/C_g^2\right) - 3.$$

Newton's law derivation: continuity and momentum equations

Simpler case: one charge, no magnetic field (general case similar)

$$\mathbf{B}_{ex} = 0, \quad \mathbf{E}_{ex} = -\nabla \varphi_{ex}, \tilde{\nabla} = \nabla$$

NLS takes the form

$$i\hbar \partial_t \psi^\ell = -\frac{\hbar^2}{2m^\ell} \nabla^2 \psi^\ell + q\varphi_{ex} \psi^\ell + \frac{\hbar^2}{2m^\ell} G_a' \left(\left| \psi^\ell \right|^2 \right) \psi^\ell,$$

Multiplying by $i\psi^{\ell *}$ and taking real part we get continuity equation

$$\partial_t \left| \psi^\ell \right|^2 + \nabla \cdot \frac{1}{m^\ell} \mathbf{P}^\ell = 0,$$

where momentum density

$$\mathbf{P}^\ell = \frac{i\hbar}{2} \left(\psi^\ell \nabla \psi^{\ell *} - \psi^{\ell *} \nabla \psi^\ell \right).$$

Let

$$\mathsf{P}^\ell = \int_{\mathbb{R}^3} \mathbf{P}^\ell d\mathbf{x},$$

We multiply NLS by $\nabla \psi^{\ell *}$ take the real part, integrate and obtain

$$\frac{d\mathsf{P}^\ell}{dt} = q^\ell \int_{\mathbb{R}^3} \mathbf{E}_{ex} \left| \psi^\ell \right|^2 \, d\mathbf{x}$$

Newton's law derivation

Define center of distribution as

$$\mathbf{r}^{\ell}(t) = \mathbf{r}_a^{\ell}(t) = \int_{\mathbb{R}^3} \mathbf{x} \left|\psi_a^{\ell}(t, \mathbf{x})\right|^2 d\mathbf{x}, \ ,$$

Multiply continuity equation by $\mathbf{x}$,

$$\mathbf{x}\partial_t \left|\psi^{\ell}\right|^2 + \mathbf{x}\nabla \cdot \frac{1}{m^{\ell}}\mathbf{P}^{\ell} = 0,$$

integrate

$$\frac{d\mathbf{r}^{\ell}(t)}{dt} = -\frac{1}{m^{\ell}} \int \mathbf{x}\nabla \cdot \mathbf{P}^{\ell} dx = \frac{1}{m^{\ell}} \int \mathbf{P}^{\ell} dx = \frac{1}{m^{\ell}} \mathsf{P}^{\ell}.$$

Combining with $\frac{d\mathsf{P}^{\ell}}{dt} = q^{\ell} \int_{\mathbb{R}^3} \mathbf{E}_{ex} \left|\psi^{\ell}\right|^2 d\mathbf{x}$ we get

$$\frac{d^2}{dt^2}\mathbf{r}^{\ell}(t) = \frac{q^{\ell}}{m^{\ell}}\mathbf{E}_{ex}\left(\mathbf{r}^{\ell}\right) + \int_{\mathbb{R}^3} \left(\mathbf{E}_{ex}(\mathbf{x}) - \mathbf{E}_{ex}\left(\mathbf{r}^{\ell}\right)\right) \left|\psi^{\ell}\right|^2 d\mathbf{x}$$

Localization assumption:

$$\int_{\mathbb{R}^3} \left(\mathbf{E}_{ex}(\mathbf{x}) - \mathbf{E}_{ex}\left(\mathbf{r}^{\ell}\right)\right) \left|\psi_a^{\ell}\right|^2 d\mathbf{x} \to \mathbf{0} \quad \text{as} \quad a \to 0$$

If *localization assumption holds* , we obtain in the limit Newton's law

$$\frac{d^2}{dt^2}\mathbf{r}^{\ell}(t) = \frac{q^{\ell}}{m^{\ell}}\mathbf{E}_{ex}\left(\mathbf{r}^{\ell}\right)$$

Exact wave-corpuscle solutions (accelerating solitons)

Let us assume a purely electric external EM field: $\mathbf{A}_{ex}=0$, $\mathbf{E}_{ex}(t,\mathbf{x})=-\nabla\varphi_{ex}(t,\mathbf{x})$.
We define the *wave-corpuscle* (soliton) ψ,φ by

$$\psi(t,\mathbf{x})=e^{iS/\hbar}\mathring{\psi}_a(|\mathbf{x}-\mathbf{r}|), \qquad S=m\mathbf{v}(t)\cdot(\mathbf{x}-\mathbf{r})+s_p(t),$$
$$\mathbf{r}=\mathbf{r}(t), \qquad \mathbf{v}(t)=\frac{d\mathbf{r}}{dt},$$

where $\mathring{\psi}_a$ is a ground state,
$\mathbf{r}(t)$ is determined from Newton's law, $s_p(t)$ is a phase shift

$$m\frac{d^2\mathbf{r}(t)}{dt^2}=q\mathbf{E}_{ex}(t,\mathbf{r}),$$

If $\mathbf{E}_{ex}(t,\mathbf{x})$ is linear in $\mathbf{x}$ then wave-corpuscle is an exact solution to NLS (accelerating soliton). We have

$$|\psi(t,\mathbf{x})|^2=a^{-3}\left|\mathring{\psi}_a\left(a^{-1}|\mathbf{x}-\mathbf{r}|\right)\right|^2\to\delta(\mathbf{x}-\mathbf{r})$$

and it satisfies *for regular enough* $\mathbf{E}_{ex}(\mathbf{x})$ the localization assumption:

$$\int_{\mathbb{R}^3}\left(\mathbf{E}_{ex}(\mathbf{x})-\mathbf{E}_{ex}\left(\mathbf{r}^\ell\right)\right)\left|\psi_a^\ell\right|^2 d\mathbf{x}\to\mathbf{0} \quad \text{as} \quad a\to 0$$

Non-relativistic electron-proton system

A system with $N=2$ charges where indices ℓ take two values $\ell=1$ (electron) and $\ell=2$ (proton). The charges have opposite values $q_1=-q_2=-q$ and masses m_1, m_2

$$\frac{\hbar}{q^2} i\partial_t \psi_1 + \frac{a_1}{2}\nabla^2 \psi_1 + \Phi_2 \psi_1 = \frac{a_1}{2} G_1' \left(|\psi_1|^2\right)\psi_1,$$

$$\frac{\hbar}{q^2} i\partial_t \psi_2 + \frac{a_2}{2}\nabla^2 \psi_2 + \Phi_1 \psi_2 = \frac{a_2}{2} G_2' \left(|\psi_2|^2\right)\psi_2,$$

$$\nabla^2 \Phi_1 = -4\pi |\psi_1|^2, \qquad \nabla^2 \Phi_2 = -4\pi |\psi_2|^2.$$

Notations

$$\Phi_1 = \varphi_1/q_1, \qquad \Phi_2 = \varphi_2/q_2,$$

$$a_1 = \frac{\hbar^2}{q^2 m_1}, \qquad a_2 = \frac{\hbar^2}{q^2 m_2}.$$

The constant a_1 coincides with Bohr radius for hydrogen if m_1 and q is electron mass and charge. The parameter

$$b = \frac{a_2}{a_1} = \frac{m_1}{m_2} \simeq \frac{1}{1837} \ll 1$$

for electron-proton. The size parameter $a = a^{(\ell)}$ in nonlinearities G_ℓ' is different for electron and proton.

Energy and charge

Charge conservation for solutions:

$$\int |\psi_1|^2 \, d\mathbf{x} = 1, \int |\psi_2|^2 \, d\mathbf{x} = 1$$

The energy

$$\begin{aligned} \boldsymbol{\mathcal{E}}(\psi_1, \psi_2) =& q^2 \int \left[\frac{a_1}{2} |\nabla \psi_1|^2 + \frac{a_1}{2} G_1 \left(|\psi_1|^2 \right) - 4\pi |\psi_1|^2 \left(-\nabla^2 \right)^{-1} |\psi_2|^2 \right] \, d\mathbf{x} \\ &+ q^2 \int \left[\frac{a_2}{2} |\nabla \psi_2|^2 + \frac{a_2}{2} G_2 \left(|\psi_2|^2 \right) \right] d\mathbf{x}, \end{aligned}$$

Energy conservation for solutions:

$$\frac{d}{dt} \boldsymbol{\mathcal{E}}(\psi_1, \psi_2) = 0$$

Multiharmonic solutions for electron-proton

Electric potentials Φ_1, Φ_2 of a resting atom should be *time independent* , hence $|\psi_1|^2, |\psi_2|^2$ do not depend on time. Hence we assume that

$$\psi^{\ell}(t,\mathbf{x}) = e^{-i\omega_{\ell}t}\psi_{\ell}(\mathbf{x}), \qquad ,\ell = 1,2.$$

and obtain *nonlinear eigenvalue problem*

$$\frac{\hbar}{q^2}\omega_1\psi_1 + \frac{a_1}{2}\nabla^2\psi_1 + \Phi_2\psi_1 = \frac{a_1}{2}G_1'\left(|\psi_1|^2\right)\psi_1,$$

$$\frac{\hbar}{q^2}\omega_2\psi_2 + \frac{a_2}{2}\nabla^2\psi_2 + \Phi_1\psi_2 = \frac{a_2}{2}G_2'\left(|\psi_2|^2\right)\psi_2.$$

Multiharmonic solutions ψ_1, ψ_2 are *critical points* of $\mathcal{E}(\psi_1,\psi_2)$ with constraint $\|\psi_{\ell}\|^2 = 1$, $\frac{\hbar}{q^2}\omega_{\ell}$ are Lagrange multipliers. Similar problems studied by Berestycki and Lions (1983), Lions (1987) have discrete eigenvalues.

If the nonlinearities G_1', G_2' are logarithmic, then for any two multi-harmonic solutions *Planck-Einstein frequency-energy relation holds* :

$$\mathsf{E}_{0\ell} - \mathsf{E}_{0\ell}' = \hbar\left(\omega_{\ell} - \omega_{\ell}'\right) \qquad \ell = 1,...,N.$$

where $\ell-$th charge energy in the system

$$\mathsf{E}_{0\ell} = \int q^{\ell}|\psi^{\ell}|^2\varphi_{\neq\ell}\,d\mathbf{x} + \frac{q^2 a_{\ell}}{2}\int \frac{\hbar^2}{2m^{\ell}}\left\{|\nabla\psi^{\ell}|^2 + G^{\ell}\left(|\psi^{\ell}|^2\right)\right\}\,d\mathbf{x}.$$

We take logarithmic nonlinearity. We study *lower critical energy levels and frequencies* ω_1 of electron to show that they are close to hydrogen atom energy levels.

Reduction of the hydrogen system

Change of variables

$$\mathbf{x} = a_\ell \mathbf{y}_\ell, \qquad \ell = 1, 2,$$

and rescale the fields as follows:

$$\Phi_\ell(\mathbf{x}) = \frac{\phi_\ell(\mathbf{y}_\ell)}{a_\ell}, \qquad \psi_\ell(\mathbf{x}) = \frac{1}{a_\ell^{3/2}} \Psi_\ell(\mathbf{y}_\ell), \ell = 1, 2.$$

Hence we obtain the following *nonlinear hydrogen system*

$$\frac{\hbar a_1}{q^2}\omega_1 \Psi_1 + \frac{1}{2}\nabla^2 \Psi_1 + \frac{1}{b}\phi_2\left(\frac{\mathbf{y}}{b}\right)\Psi_1 = \frac{1}{2}G_1'\left(|\Psi_1|^2\right)\Psi_1,$$

$$\frac{\hbar a_2}{q^2}\omega_2 \Psi_2 + \frac{1}{2}\nabla^2 \Psi_2 + b\phi_1(b\mathbf{y})\Psi_2 = \frac{1}{2}G_2'\left(|\Psi_2|^2\right)\Psi_2.$$

$$\nabla_{\mathbf{y}}^2 \phi_1 = -4\pi |\Psi_1|^2, \qquad \nabla_{\mathbf{y}}^2 \phi_2 = -4\pi |\Psi_2|^2.$$

Reduction to one charge in the Coulomb field

To find energy levels and frequences consider *radial solutions* $\Psi_1(r), \Psi_2(r)$.
Note that the electron/proton mass ratio $\frac{m_1}{m_2} \simeq \frac{1}{1837}$ is small, therefore the parameter

$$b = \frac{a_2}{a_1} = \frac{m_1}{m_2} \simeq \frac{1}{1837} \ll 1,$$

we consider $b \to 0$. Interaction contribution to energy

$$\int b\phi_1(b\mathbf{y}) |\Psi_2|^2 d\mathbf{y} \to 0$$

$$D = -\int \left(\frac{1}{b}\phi_2\left(\frac{1}{b}\mathbf{y}_1\right) - \frac{1}{|\mathbf{y}_1|} \right) |\Psi_1|^2 d\mathbf{y}_1 = \tag{1}$$

$$= 4\pi \int_0^\infty \frac{4\pi}{r} |\Psi_1(r)|^2 r^2 \int_{r/b}^\infty (r_1 - r/b) r_1 |\Psi_2(r_1)|^2 dr_1 dr.$$

$$|D| \leq \frac{(4\pi)^2}{6} b^2 \max_r |\Psi_1(r)|^2 \int_0^\infty |\Psi_2(r_1)|^2 r_1^4 dr_1,$$

To estimate lower critical energy levels of $\mathcal{E}(\psi_1, \psi_2)$ if $b \to 0$ we replace $b\phi_1(b\mathbf{y})$ by 0 and $\frac{1}{b}\phi_2\left(\frac{\mathbf{y}}{b}\right)$ by Coulomb potential $\frac{1}{|\mathbf{y}|}$ and consider for $\|\Psi_1\| = 1, \|\Psi_2\| = 1$ reduced $b \to 0$ energy

$$\mathcal{E}_0(\psi_1, \psi_2) = \mathcal{E}_{Cb}(\Psi_1) + \mathcal{E}(\Psi_2),$$

$$\mathcal{E}(\Psi_2) = \frac{q^2}{a_2\hbar} \int_{\mathbb{R}^3} \left[\frac{1}{2} |\nabla\Psi_2|^2 + \frac{1}{2} G_2\left(|\Psi_2|^2\right) \right] d\mathbf{y}$$

(Reduction similar to Born-Oppenheimer approximation.) The lower critical levels of $\mathcal{E}_0(\psi_1, \psi_2)$ are given by

$$\min_{\|\Psi_2\|=1} \mathcal{E}(\Psi_2) + E_n^{\kappa,\xi}$$

where $E_n^{\kappa,\xi}$ are the lower critical levels on $\|\Psi_1\| = 1$ of

$$\mathcal{E}_{Cb}(\Psi_1) = \frac{q^2}{a_1\hbar} \int_{\mathbb{R}^3} \left[\frac{1}{2} |\nabla\Psi_1|^2 + \frac{1}{2} G_1\left(|\Psi_1|^2\right) - \frac{1}{|\mathbf{y}|} |\Psi_1|^2 \right] d\mathbf{y}.$$

See details in Babin, Figotin DCDS (2010).

Lower energy levels of nonlinear hydrogen model with Coulomb potential

Consider (using dimensionless variable $\mathbf{y} = \mathbf{y}_1$)

$$\mathcal{E}_{Cb}(\Psi_1) = \frac{q^2}{a_1 \hbar} \int_{\mathbb{R}^3} \left[\frac{1}{2} |\nabla \Psi_1|^2 + \frac{1}{2} G_1\left(|\Psi_1|^2\right) - \frac{1}{|\mathbf{y}|} |\Psi_1|^2 \right] d\mathbf{y}.$$

with logarithmic nonlinearity

$$G_1\left(|\Psi|^2\right) = -\kappa^2 |\Psi|^2 \left(\ln\left(\kappa^{-3} |\Psi|^2 / C_g^2\right) + 2\right)$$

Theorem (Babin, Figotin DCDS (2010)). Lower critical levels of $\mathcal{E}_{Cb}(\Psi_1)$ on $\|\Psi_1\| = 1$

$$\mathcal{E}_{Cb}(\Psi_1) = \frac{q^2}{a_1 \hbar} \int_{\mathbb{R}^3} \left[\frac{1}{2} |\nabla \Psi_1|^2 + \frac{1}{2} G_1\left(|\Psi_1|^2\right) - \frac{1}{|\mathbf{y}|} |\Psi_1|^2 \right] d\mathbf{y}.$$

satisfy the estimate

$$\left|E_n^\kappa - E_n^0\right| \leq C_N \frac{q^2}{a_1 \hbar} \left(\kappa^2 |\ln \kappa|\right), \quad n = 1, ..., N$$

where E_n^0 are linear hydrogen Schrodinger operator energy levels as in quantum mechanics:

$$E_n^0 = -\frac{q^2}{a_1 \hbar} \frac{1}{2n^2}, \; n = 1, 2, ..$$

$$\kappa = \frac{a_1}{a}$$

$a_1 \simeq 53 \times 10^{-3}$ nanometers is Bohr radius.

Observation: For macroscopic scales R if size factor a is small, $\frac{a}{R} << 1$ we obtain Newtonian dynamics with Lorentz force.. At atomic scales, if $\frac{a}{a_1} >> 1$ we obtain classical spectral structure of hydrogen energy levels as in Bohr and Schrodinger models. Hence scale restrictions are:

$$a_1 << a << R$$

Note that Bohr radius $a_1 \sim 5.29 \times 10^{-11}$ meters which leaves a space for macroscopic scales R and for electron size parameter a

Dynamical description of transitions. Semi-relativistic model

Reduced non-relativistic model with Coulomb potential

$$\frac{\hbar a_1}{q^2} i\partial_t \Psi_1 + \frac{1}{2}\nabla^2 \Psi_1 + \phi_2 \Psi_1 - \frac{1}{2} G'_{1,a}\left(|\Psi_1|^2\right)\Psi_1 = 0$$

$$\nabla^2_{\mathbf{y}} \phi_2 = -4\pi\delta\left(\mathbf{y}\right)$$

$$\|\Psi_1\| = 1$$

has multiharmonic solutions representing hydrogen atom states. Oversimplified to describe transitions. Hence we introduce reduced semi-relativistic model

Electron in Coulomb field

$$\frac{\hbar a_1}{q^2} i\partial_t \psi_1 + \frac{1}{2}\nabla^2 \psi_1 + \left(\frac{1}{|y|} + \eta\phi\right)\psi_1 - \frac{1}{2} G'_1\left(|\psi_1|^2\right)\psi_1 = 0$$

with *self-coupling* with electric potential (similar to Babin, Figotin J. Stat. Phys. 2010), coefficient η with $|\eta| << 1$ controls the self-coupling

$$-\frac{a_1^2}{c^2}\partial_t^2 \phi + \nabla^2 \phi = -4\pi\eta\left|\psi_1\right|^2$$

Energy conservation

$$\boldsymbol{\mathcal{E}}\left(\psi,\phi\right) = \frac{q^2}{\hbar a_1}\left[\int \frac{1}{2}\left|\nabla\psi_1\right|^2 - \frac{1}{|x|}\left|\psi_1\right|^2 - \eta\phi\left|\psi_1\right|^2 + \frac{1}{2} G_1\left(|\psi_1|^2\right) dy + \frac{1}{4\pi}\int\left(\frac{1}{2c^2}\left|\partial_t\phi\right|^2 + \frac{1}{2}\left|\nabla\phi\right|^2\right) dy\right]$$

$$\partial_t \boldsymbol{\mathcal{E}}\left(\psi,\phi\right) = 0$$

Multiharmonic solutions are close to non-relativistic as $\eta \to 0$. Allows in principle radiation and transitions between energy levels. Self-coupling allows for energy transfer from single charge to electric field with subsequent radiation.

Semi-relativistic model with damping

Electron in Coulomb field

$$\frac{\hbar}{q^2} i\partial_t \psi + \frac{1}{2}\nabla^2\psi + \left(\frac{1}{|y|} + \eta\Phi\right)\psi - \frac{1}{2}G_1'\left(|\psi|^2\right)\psi = 0$$

Wave equation with damping for potential Φ

$$\left(-\frac{a_1^2}{c^2}\partial_t^2\Phi - \frac{\kappa_0 a_1}{c}\partial_t\Phi + \nabla^2\Phi\right) = -4\pi\eta\,|\psi|^2$$

where $0 < \kappa_0 << 1$. The damping models losses of energy thanks to radiative interaction with environment. Same energy $\mathcal{E}(\psi,\phi)$ but now energy is not conserved:

$$\partial_t \mathcal{E}(\psi,\Phi) = -\frac{\kappa_0 a_1}{4\pi c}\int (\partial_t\Phi)^2\,dx \leq 0$$

$$\|\psi\| = 1$$

provides (degenerate) Lyapunov functional. $\partial_t\mathcal{E} = 0$ implies $\partial_t\Phi = 0$, $\partial_t|\psi|^2 = 0$ but $\partial_t\psi$ may be non-zero as for multi-harmonic solutions, hence periodic solutions are possible. The dissipation integral

$$\mathcal{E}(T_2) - \mathcal{E}(T_1) = -\frac{\kappa_0 a_1}{4\pi c}\int_{T_1}^{T_2}(\partial_t\Phi)^2\,dt$$

can be used to find convergence to time independent Φ and $|\psi|^2$.

Attractor as dynamical model for spontaneous transitions

Hydrogen atom is modeled in this setting by *attractor* of this system restricted to the lower energy set

$$\left\{ \|\psi\| = 1, \boldsymbol{\mathcal{E}}\left(\psi, \Phi\right) \leq E \right\}$$

with a fixed $E < 0$. ($E < 0$ corresponds to discrete spectrum). This is a *dynamical model* of transitions compared with statistical model in quantum mechanics. The attractor contains *multi-harmonic periodic solutions* and connecting orbits Spontaneous transitions from higher energy multi-harmonic states to lower energy can be modeled as dynamics on the attractor.

Interesting problems:

To give precise meaning of attraction to the attractor, study limits $a \to 0, \kappa_0 \to 0$.

Structure of the attractor.

Case of radial ψ : it is simpler in many respects, but still non-trivial. Time independent $|\psi|^2$ imply that ψ is harmonic.

Wave equation with a stronger damping for potential Φ

$$-\frac{a_1^2}{c^2}\partial_t^2\Phi + \frac{L_0 a_1}{c}\nabla^2\partial_t\Phi + \nabla^2\Phi = -4\pi\eta\left|\psi\right|^2$$

with $L_0 << 1$ may be easier to study.

Relativistic dynamics of a single point

A single particle in an external EM field is governed by the Klein-Gordon equation

$$-\frac{1}{c^2}\tilde{\partial}_t\tilde{\partial}_t\psi + \tilde{\nabla}^2\psi - G'(\psi^*\psi)\,\psi - \kappa_0^2\psi = 0$$

where the external field potentials $\varphi_{ex}, \mathbf{A}_{ex}$, which are assumed to be known functions of $(t, \mathbf{x})$, enter through covariant derivatives:

$$\tilde{\partial}_t = \partial_t + \frac{iq\varphi_{ex}}{\hbar},\ \tilde{\nabla} = \nabla - \frac{iq\mathbf{A}_{ex}}{\hbar c},$$

and the coefficient κ_0 has the form

$$\kappa_0 = \frac{mc}{\hbar}$$

where m is the mass parameter, c is speed of light and $\hbar$ is Planck constant. The Lagrangian for Klein-Gordon equation

$$\mathcal{L}_1(\psi) = \frac{\hbar^2}{2m}\left\{\frac{1}{c^2}\left(\tilde{\partial}_t\psi\tilde{\partial}_t^*\psi^*\right) - \left(\tilde{\nabla}\psi\tilde{\nabla}^*\psi^*\right) - \kappa_0^2\psi^*\psi - G(\psi^*\psi)\right\}.$$

Energy, charge and momentum

The definition of *charge energy density* is derived from the Lagrangian $\mathcal{L}_1(\psi)$ in a standard way,

$$E_{pt} = \frac{\hbar^2}{2m}\left(\frac{1}{c^2}\left(\tilde{\partial}_t\psi\tilde{\partial}_t^*\psi^*\right) + \left(\tilde{\nabla}\psi\tilde{\nabla}^*\psi^*\right) + G\left(\psi^*\psi\right) + \kappa_0^2\psi\psi^*\right).$$

Similarly, we define the *relativistic charge momentum density* by the formula

$$\mathbf{P}_{rel} = -\frac{\hbar^2}{2mc^2}\left(\tilde{\partial}_t\psi\tilde{\nabla}^*\psi^* + \tilde{\partial}_t^*\psi^*\tilde{\nabla}\psi\right).$$

We denote

$$\mathbf{P} = \frac{\hbar}{2i}\left(\psi^*\tilde{\nabla}\psi - \psi\tilde{\nabla}^*\psi^*\right) = \hbar\, Im\,\frac{\tilde{\nabla}\psi}{\psi}\left|\psi\right|^2$$

and call $\mathbf{P}$ *non-relativistic charge momentum density* .

We denote

$$\rho = \frac{q\hbar}{mc^2}\frac{1}{2i}\left(\tilde{\partial}_t^*\psi^*\psi - \tilde{\partial}_t\psi\psi^*\right) = -\frac{q\hbar}{mc^2}\left(Im\,\frac{\partial_t\psi}{\psi} + \frac{q\varphi_{ex}}{\hbar}\right)\left|\psi\right|^2$$

and call it *charge density* .

We also introduce spatial averages

$$\bar{\rho} = \int \rho d^3x,\ \ \bar{\mathbf{P}}_{rel} = \int \bar{\mathbf{P}}_{rel} d^3x,\ \ \bar{\mathbf{P}} = \int \mathbf{P} d^3x,\ \ \bar{E}_{pt} = \int E_{pt} d^3x.$$

Ergocenter is defined by the formula

$$\mathbf{r}\left(t\right) = \frac{1}{\bar{E}_{pt}}\int_{\mathbb{R}^3}\mathbf{x}E_{pt}d\mathbf{x},\quad \bar{E}_{pt} = \int_{\mathbb{R}^3}E_{pt}d\mathbf{x}.$$

Ergocenter integral equations

From continuity equation we obtain

$$\partial_t \bar{\rho} = 0$$

and we assume Coulomb normalization

$$\bar{\rho} = q$$

Some manipulation with the equations (multiplication, integration by parts etc.) produces two more ergocenter equations

$$\partial_t \bar{E}_{pt} = \partial_t \mathbf{r} \cdot \mathbf{E}_{ex} (\mathbf{r}) \bar{\rho} + R_E,$$
$$R_E = \partial_t \mathbf{r} \cdot \int (\mathbf{E}_{ex} (\mathbf{x}) - \mathbf{E}_{ex} (\mathbf{r})) \rho d\mathbf{x} + \partial_t \int \mathbf{E}_{ex} \cdot (\mathbf{x} - \mathbf{r}) \rho dx$$
$$- \int \partial_t \mathbf{E}_{ex} \cdot (\mathbf{x} - \mathbf{r}) \rho dx - \frac{q}{m} \int ((\mathbf{x} - \mathbf{r}) \cdot \mathbf{P}) \nabla \cdot \mathbf{E}_{ex} dx.$$

We call this equation *the first ergocenter integral equation.* The *second ergocenter integral equation* has the form

$$\frac{1}{c^2} \partial_t \left(\bar{E}_{pt} \partial_t \mathbf{r} \right) - \mathbf{E}_{ex} (\mathbf{r}) \bar{\rho} - \frac{1}{c} \partial_t \mathbf{r} (t) \times \mathbf{B}_{ex} (\mathbf{r}) \bar{\rho} + \mathbf{R}_1 = 0,$$
$$\mathbf{R}_1 = \frac{1}{c^2} \partial_t^2 \int ((\mathbf{x} - \mathbf{r}) E_{pt}) dx - \frac{q}{mc^2} \partial_t \int (\mathbf{x} - \mathbf{r}) \mathbf{E}_{ex} \cdot \mathbf{P} dx - \frac{1}{c} \partial_t \int (\mathbf{x} - \mathbf{r}) \times \mathbf{B}_{ex} \rho d\mathbf{x}$$
$$- \int (\mathbf{E}_{ex} (\mathbf{x}) - \mathbf{E}_{ex} (\mathbf{r})) \rho dx - \frac{1}{c} \partial_t \mathbf{r} (t) \times \int (\mathbf{B}_{ex} (\mathbf{x}) - \mathbf{B}_{ex} (\mathbf{r})) \rho d\mathbf{x} + \frac{q\hbar}{mc} \int ((\mathbf{x} - \mathbf{r}) \cdot \mathbf{P}) \nabla \times \mathbf{B}_{ex} d\mathbf{x}$$

Localization assumption: ρ and $\mathbf{P}$ are localized near ergocenter $\mathbf{r}$ as $a \to 0$ namely

$$\mathbf{R}_1 \to 0, R_E \to 0$$

Relativistic point dynamics in localization limit

If the localization holds, we obtain in the limit from the second ergocenter integral equation

$$\frac{1}{c^2}\partial_t\left(\bar{E}_{pt}\partial_t\mathbf{r}\right)=\mathbf{f},$$

where $\mathbf{f}$ coincides with Lorentz force

$$\mathbf{f}=q\mathbf{E}_{ex}\left(\mathbf{r}\right)+q\frac{1}{c}\partial_t\mathbf{r}\left(t\right)\times\mathbf{B}_{ex}\left(\mathbf{r}\right)$$

Equivalently we write it as Newton's law

$$\partial_t\left(\frac{\bar{E}_{pt}}{c^2}\partial_t\mathbf{r}\right)=\mathbf{f},$$

and we see that the coefficient $\frac{\bar{E}_{pt}}{c^2}=M$ plays the role of *inertial mass.* Hence Einstein formula holds

$$M=\frac{\bar{E}_{pt}}{c^2}$$

The first ergocenter integral equation produces

$$\partial_t\bar{E}_{pt}=\partial_t\mathbf{r}\cdot\mathbf{E}_{ex}\left(\mathbf{r}\right)q$$

From the system of two equation we derive the following conservation law

$$\frac{M^2\left(\partial_t\mathbf{r}\right)^2}{2c^2}-\frac{M^2}{2}=const$$

which produces familiar formula from special relativity

$$M=\gamma M_0,\gamma=\left(1-\frac{\left(\partial_t\mathbf{r}\right)^2}{c^2}\right)^{-1/2}$$

where γ is Lorentz factor.