Simulation of the Maxwell-Dirac and Schrödinger-Poisson systems

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- Introduction to the Dirac equation
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The Dirac equation

An equation for the electron, consistent with both special relativity and quantum mechanics (Paul Dirac, 1928).

Predicted the existence of antiparticles. Positrons were discovered experimentally by Carl D. Anderson in 1932.

Quantum mechanics

The Schrödinger equation:

$$E\psi = H\psi$$

Wavefunction: ψ, probability density $|\psi|^2$

Energy operator: $E = i\hbar\frac{\partial}{\partial t}$

Momentum operator: $p = -i\hbar\nabla$

Hamiltonian: $H = T + V$, e.g. $T = -\frac{p^2}{2m}$

Special relativity

Relativistic energy-momentum relation:

$$E^2 = c^2 p^2 + m^2 c^4 \tag{1}$$

Schrödinger equation + (1) = Klein-Gordon equation:

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi - \nabla^2\psi + \frac{m^2c^2}{\hbar^2}\psi = 0$$

KG is correct, but not sufficient.

The Dirac equation

The free Dirac operator (free Dirac Hamiltonian):

$$H_0 = c\alpha \cdot p + \beta mc^2 = -i\hbar c\alpha \cdot \nabla + \beta mc^2$$

$$\beta = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix}$$

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}; \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Dirac wavefunction (Dirac spinor): $(\psi_1, \psi_2, \psi_3, \psi_4)^T \in \mathbb{C}^4$,
$|\psi|^2 = \sum_{k=1}^{4} |\psi_k|^2$.

The Dirac equation with a potential

Same form as the Schrödinger equation, with Hamiltonian $H_0 + V$:

$$E\psi = (H_0 + V)\psi$$

Electrostatic potential: $V = \phi \mathbb{I}_4$

Coulomb potential: $\phi = \frac{C}{|x|}$

More generally (electromagnetic): 4×4 matrix

Spectrum of the free Dirac operator

Continuous spectrum: $(-\infty, -mc^2] \cup [mc^2, \infty)$.

In the $p \to 0$ limit, $H_0 \to mc^2\beta$, eigenvalues: $\pm mc^2$ (relativistic rest energy).

Upper (positive, electronic) and lower (negative, positronic) parts of wavefunction:

$$\psi_+ = \begin{pmatrix} \psi_1 \\ \psi_2 \\ 0 \\ 0 \end{pmatrix} \qquad \psi_- = \begin{pmatrix} 0 \\ 0 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

Dirac wavefunction: superposition of an electron and a positron.

Spectrum of the Dirac operator a potential

Coulomb potential: discrete set of eigenvalues appears in the gap.

Periodic potential: countable set of continuous intervals.

General potential: difficult!

Time evolution

Time-dependent Schrödinger (or Dirac) equation: $i\hbar\psi' = H\psi$

Formal solution: $\psi(t) = e^{-iHt/\hbar}\psi(0)$

Operator exponential:

$$e^A = \sum_{k=0}^{\infty} \frac{A^k}{k!}$$

Stone's theorem (H self-adjoint): $U(t) = e^{-iHt/\hbar}$ unitary, $U(t_1 + t_2) = U(t_1)U(t_2)$, strongly continuous with respect to t.

Time evolution of the Dirac equation

H_0 is (essentially) self-adjoint, so Stone's theorem gives existence of uniqueness for the free Dirac equation.

$H_0 + V$ remains self-adjoint (subject to some regularity conditions on V)

Coulomb potential: works as long as C is not too large.

Maxwell-Dirac equations

Coupling the Dirac equation to the generated electromagnetic field:

$$i\hbar \frac{\partial}{\partial t}\psi = \left(-i\hbar c\alpha \cdot \nabla + mc^2\beta - q\alpha \cdot (\mathbf{A} + \mathbf{A}_{\text{ex}}) + (V + V_{\text{ex}})\right)\psi$$

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta\right) V = \frac{1}{4\pi\epsilon_0}\rho$$

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta\right) \mathbf{A} = \frac{1}{4\pi\epsilon_0 c}\mathbf{J}$$

where $\rho = q|\psi|^2$ and $J_k = qc\langle \psi, \alpha_k \psi\rangle_{\mathbb{C}^4}$

Maxwell-Dirac equations (dimensionless)

$$i\epsilon \frac{\partial}{\partial t}\psi = \left(-\frac{i\epsilon}{\delta}\alpha \cdot \nabla + \frac{1}{\delta^2}\beta - \alpha \cdot (\mathbf{A} + \mathbf{A}_{\text{ex}}) + (V + V_{\text{ex}}) \right) \psi$$

$$\left(\delta^2 \frac{\partial^2}{\partial t^2} - \Delta \right) V = \epsilon |\psi|^2$$

$$\left(\delta^2 \frac{\partial^2}{\partial t^2} - \Delta \right) A_k = \epsilon \langle \psi, \alpha_k \psi \rangle$$

Semiclassical limit ($\hbar \to 0$): $\epsilon \to 0$
Nonrelativistic limit ($c \to \infty$): $\delta \to 0$

Asymptotics of the Maxwell-Dirac system

Reduction to simpler systems:

$\delta \to 0 \quad (c \to \infty)$: Schrödinger-Poisson system

$\epsilon \to 0 \quad (\hbar \to 0)$: Vlasov-Maxwell system, WKB analysis

$\delta \to 0, \epsilon \to 0$: Vlasov-Poisson system

The nonrelativistic limit

Set $\epsilon = 1$, let $\delta \to 0$. Leading-order behavior:

$$i\psi' = \frac{1}{\delta^2}\beta\psi + O\left(\frac{1}{\delta}\right)\psi$$

Solution of the leading-order equation:

$$\psi_{1,2}(t) = e^{-it/\delta^2}\psi_{1,2}(0)$$

$$\psi_{3,4}(t) = e^{+it/\delta^2}\psi_{3,4}(0).$$

Rapid phase oscillation, components do not interact.

The nonrelativistic limit (2)

Let $H = H_T + H_V$, H_T δ-scaled free Dirac operator.

Fourier transform (Fourier / momentum coordinate ξ):

$$H_T = \left(\frac{1}{\delta}\right) \alpha \cdot \xi + \frac{1}{\delta^2} \beta$$

Diagonalize H_T in Fourier space: $H_T = PDP^{-1}$.

The nonrelativistic limit (3)

Eigenvalues of H_T: $(\lambda, \lambda, -\lambda, -\lambda)$ where

$$\lambda = \frac{1}{\delta^2}\sqrt{1 + \delta^2 |\xi|^2}.$$

So H_T, up to a change of basis, equals

$$D = \beta\lambda.$$

The series expansion $\sqrt{1+x} = 1 + \frac{1}{2}x + \ldots$ gives

$$D = \beta\left(\frac{1}{\delta^2} + \frac{|\xi|^2}{2}\right) + O(\delta^2).$$

The nonsingular term is the "ordinary Schrödinger equation Hamiltonian" $\mp\frac{\Delta}{2}$.

Nonrelativistic limit of Maxwell's equations

Formally letting $\delta \to 0$ gives the Poisson equation for V,

$$-\Delta V = |\psi|^2.$$

The magnetic potential turns out to behave as $O(\delta)$, so it can be dropped.

Schrödinger-Poisson equations

Ignoring the singular term, we obtain the asymptotic system:

$$i\frac{\partial}{\partial t}\phi_e = -\frac{\Delta}{2}\phi_e + (V + V_{\mathrm{ex}})\phi_e$$

$$i\frac{\partial}{\partial t}\phi_p = +\frac{\Delta}{2}\phi_p + (V + V_{\mathrm{ex}})\phi_p$$

$$-\Delta V = |\phi_e|^2 + |\phi_p|^2$$

Relation between MD and SP

When $\delta \to 0$,

$$\phi_e \to \psi_e = e^{it/\delta^2} \Pi_e \psi \to e^{it/\delta^2} \psi_+$$

$$\phi_p \to \psi_p = e^{-it/\delta^2} \Pi_p \psi \to e^{-it/\delta^2} \psi_-$$

Positive/negative energy subspace projection operators:

$$\Pi_e \to \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & 0 \end{pmatrix} \qquad \Pi_p \to \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{I}_2 \end{pmatrix}$$

Numerical simulation

The MD equations are a coupled system of hyperbolic differential equations, presenting considerable difficulties for numerical algorithms and simulations.

Problem 1: solving the MD and SP systems.

Problem 2: solving MD accurately for small values of δ to compare with the asymptotic solution.

Pseudospectral method for MD and SP

Huang, Jin, Markowich, Sparber & Zheng, “A time-splitting spectral scheme for the Maxwell-Dirac system”, J. Comput. Phys., 208(2):761-789, 2005.

also

Bao & Li, “An efficient and stable numerical method for the Maxwell-Dirac system”. J. Comput. Phys., 199(2):663-687, 2004.

Numerical method

Method for a general Schrödinger-type equation

$$i\psi' = H\psi \qquad H = T + V$$

where T can be diagonalized in Fourier (momentum) space, V can be diagonalized in ordinary space.

$$e^{-i\tau H} \approx e^{-i\tau V} e^{-i\tau T}$$

$$\psi(t+\tau) = e^{-i(T+V)\tau}\psi_0 \approx \mathcal{F}^{-1}\left(e^{-iT\tau}\mathcal{F}\left(e^{-iV\tau}\psi(t)\right)\right).$$

The pseudospectral method

Fourier series on $[-L/2, L/2]$

$$f(x) = \sum_{k=-\infty}^{\infty} c_k \phi_k(x) \quad \approx \quad f_N(x) = \sum_{k=-N/2+1}^{N/2} c_k \phi_k(x)$$

$$c_k = \frac{1}{2L} \int_0^{2L} f(x)\overline{\phi_k(x)}dx$$

$$\phi_k(x) = e^{2\pi ikx/L}$$

Choose uniform sample points, trapezoidal quadrature:

$$(x_0, x_1, \ldots, x_{N-1}), \quad x_k = -\frac{L}{2} + \frac{kL}{N}.$$

DFT and FFT

DFT:

$$c_k = \sum_{n=0}^{N-1} f(x_n) e^{-\frac{2\pi i}{N} kn} \qquad k = 0, \ldots, N-1$$

IDFT:

$$f(x_n) = \frac{1}{N} \sum_{k=0}^{N-1} c_k e^{\frac{2\pi i}{N} kn} \qquad n = 0, \ldots, N-1$$

DFT can be computed efficiently using FFT ($O(N \log N)$ time).

Pseudospectral method for differential equations

DFT approximates the exact Fourier transform:

$\mathcal{F}(f) \Leftrightarrow$ Fourier series coefficients from function values (DFT)

$\mathcal{F}^{-1}(\hat{f}) \Leftrightarrow$ function values from Fourier series coefficients (IDFT)

In particular, differential operators turn into multiplication by the Fourier series coefficients (Fourier space coordinates).

$$\phi_k'(x) = \frac{2\pi ik}{L}\phi_k(x) = i\xi_k\phi_k$$

$$\mathcal{F}\left(\frac{\partial}{\partial x}\right) = i\xi \qquad \mathcal{F}\left(\frac{\partial^2}{\partial x^2}\right) = -|\xi|^2$$

Pseudospectral method for Maxwell-Dirac

1. Solve $i\epsilon\psi' = -\frac{i\epsilon}{\delta}\alpha \cdot \nabla\psi + \frac{1}{\delta^2}\beta\psi$ in Fourier space
2. Solve Maxwell's equations as ODEs in Fourier space, using Crank-Nicolson time-stepping
3. Solve $i\epsilon\psi' = -\alpha \cdot (\mathbf{A} + \mathbf{A}^{ex})\psi + (V + V^{ex})\psi$ in real space

Analogous method for Schrödinger-Poisson.

First matrix exponential

Solve $i\epsilon\psi' = H_T\psi$ in Fourier space, i.e. compute $\exp(M_1)\psi = \exp(-iH_T\tau/\epsilon)\psi$.

$$M_1 = \frac{\tau}{\delta}\begin{pmatrix} -a & 0 & -i\xi_3 & -i\xi_1 - \xi_2 \\ 0 & -a & -i\xi_1 + \xi_2 & i\xi_3 \\ -i\xi_3 & -i\xi_1 - \xi_2 & a & 0 \\ -i\xi_1 + \xi_2 & i\xi_3 & 0 & a \end{pmatrix}$$

Eigenvalues $(\lambda, \lambda, -\lambda, -\lambda)$ where

$$\lambda = \frac{i\tau}{\epsilon\delta^2}\sqrt{1 + \epsilon^2\delta^2|\xi|^2}$$

Exact computation of the matrix exponential

Use diagonalization:

$$e^{M_1} = Pe^D P^{-1}$$

Let $c = \cos(\lambda/i)$, $s = \sin(\lambda/i)$, $\omega = \epsilon\delta\xi$, $t = s(1 + |\omega|^2)^{-1/2}$:

$$e^{M_1} = \begin{pmatrix} c - it & 0 & -is\omega_3 & -s(\omega_2 + i\omega_1) \\ 0 & c - it & s(\omega_2 - i\omega_1) & is\omega_3 \\ -is\omega_3 & -s(\omega_2 + i\omega_1) & c + it & 0 \\ s(\omega_2 - i\omega_1) & is\omega_3 & 0 & c + it \end{pmatrix}.$$

Similarly for the matrix in the last step.

Solving Maxwell's equations

Maxwell's equations rewritten as ODEs in Fourier space:

$$\left(\delta^2 \frac{\partial^2}{\partial t^2} + |\xi|^2\right) \widehat{V} = \epsilon \widehat{|\psi|^2}$$

$$\left(\delta^2 \frac{\partial^2}{\partial t^2} + |\xi|^2\right) \widehat{A_k} = \epsilon \langle \widehat{\psi, \alpha_k \psi} \rangle \quad k = 1, 2, 3$$

Second order ODEs, so we need both f and f' as initial conditions.

Crank-Nicolson method

Convert to a first-order, two-dimensional system:

$$g = (f, f')$$

Crank-Nicolson method for an ODE system:

$$\mathbf{R}g' + \mathbf{S}g = \mathbf{v}$$

$$g_{n+1} = \left(\mathbf{R} + \frac{\tau}{2}\mathbf{S}\right)^{-1} \left(\frac{\tau}{2}\left(\mathbf{v}_n + \mathbf{v}_{n+1}\right) + \left(\mathbf{R} - \frac{\tau}{2}\mathbf{S}\right) g_n\right)$$

Schrödinger-Poisson algorithm

$$\chi_e = \mathcal{F}^{-1}\left[\exp\left(-\frac{1}{2}i|\xi|^2\tau\right)\mathcal{F}\left[\phi_e(t)\right]\right]$$

$$\chi_p = \mathcal{F}^{-1}\left[\exp\left(\frac{1}{2}i|\xi|^2\tau\right)\mathcal{F}\left[\phi_p(t)\right]\right]$$

$$V = \mathcal{F}^{-1}\left[\frac{1*}{|\xi|^2}\mathcal{F}\left[|\chi_e|^2 + |\chi_p|^2\right]\right]$$

$$\phi_{e/p}(t+\tau) = \exp\left(-i\tau\left(V + V_{\text{ex}}\right)\right)\chi_{e/p}$$

Useful properties of the algorithm

- Probability is conserved exactly (up to roundoff).
- High spatial accuracy for smooth data.
- We solve *exactly* for the leading singular dependence on δ, so the algorithm works for small values of δ.
- Apart from the singular contribution, the MD update matrix converges to the SP update matrix in the $\delta \to 0$ limit.

Simulation results

Algorithm implemented in Matlab.

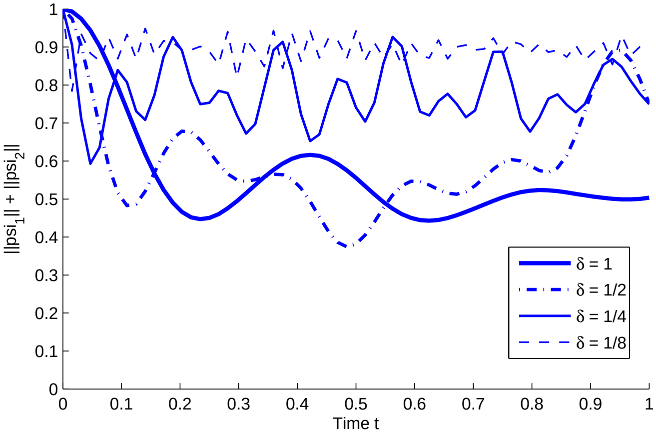
Results of some test runs on a box $[-0.5, 0.5]^3$, $32^3 - 64^3$ points.

Smooth initial data and potentials, e.g.

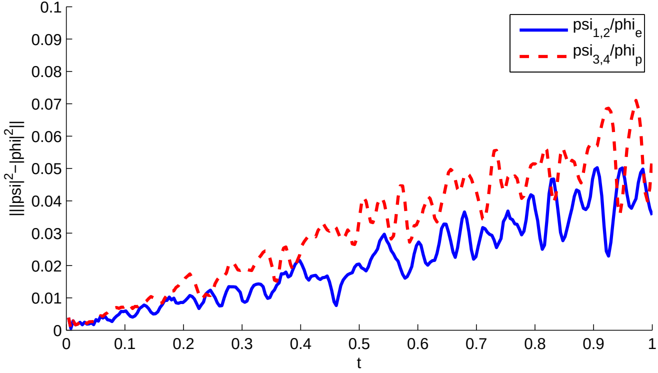
$$\psi_k = \cos^2(\pi(x + 0.1)) \cos^2(\pi(y + 0.1))$$

$$V_{\text{ex}} = 50 \sin^4(\pi x) \sin^4(\pi y)$$

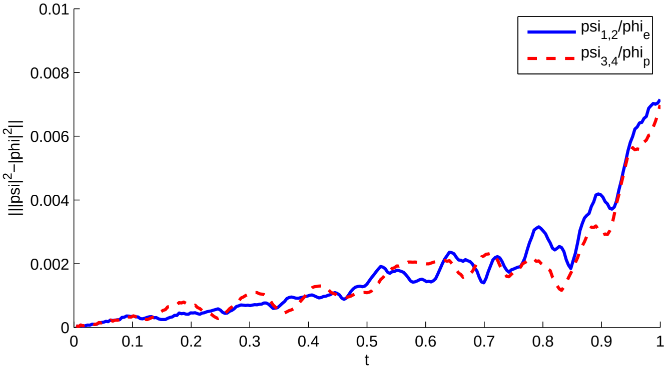
Interaction of upper and lower components



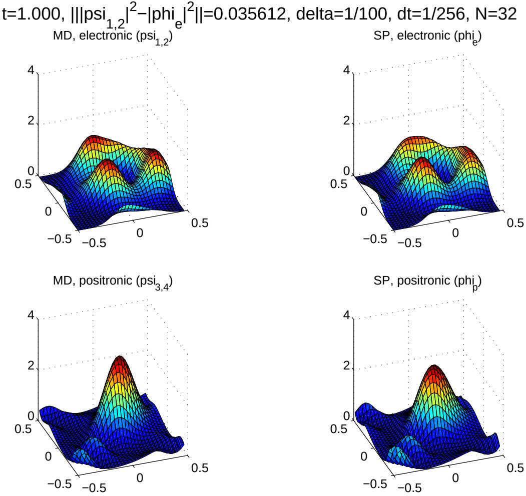
$\| |\psi_{1,2}|^2 - |\phi_e|^2 \|$, $\| |\psi_{3,4}|^2 - |\phi_p|^2 \|$, $\delta = 1/100$



$\||\psi_{1,2}|^2 - |\phi_e|^2\|$, $\||\psi_{3,4}|^2 - |\phi_p|^2\|$, $\delta = 1/1000$



Visual comparison of MD and SP



Discussion

Results from simple test problems confirm that the solver works well for MD with small δ.

Simulations verify that MD is well-approximated by SP as $\delta \rightarrow 0$.

Much more can be be investigated: choice of initial data, choice of potentials, number of space dimensions, and space/time resolution, magnetic field, ...