The Madelung Equations

A Hydrodynamic Theory of Quantum Mechanics

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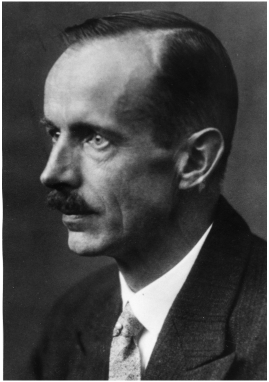
Erwin Madelung



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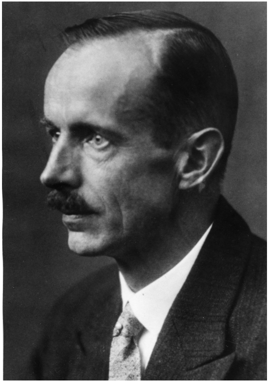
Erwin Madelung (1881 - 1972)

Madelung was a German physicist who received his doctorate from the University of Göttingen, specializing in crystal structure. In 1921, he succeeded Max Born as the Chair of Theoretical Physics at the Goethe University Frankfurt, where he worked on quantum mechanics, and developed the Madelung equations.

Erwin Madelung (cont.)



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Erwin Madelung (1881 - 1972)

Madelung discovered the Madelung equations by writing the wave function, ψ in polar form and substituting it into the Schrödinger Equation

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The Schrödinger Equation

The time dependent Schrödinger equation reads

$$i\hbar\frac{\partial}{\partial t}\left|\psi\right\rangle = \hat{H}\left|\psi\right\rangle$$

Equivalently, we can write

Time Dependent Schrödinger Equation

$$i\hbar\frac{\partial}{\partial t}\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi$$

The Madelung Transformation

Erwin Madelung, in 1926, introduced the following change of variables

Madelung Transformation

$$\psi = \sqrt{\rho} e^{\frac{i\theta}{2}}$$

- $\rho = \psi\psi^* = |\psi|^2$, $\rho \geq 0$
  Describes the density distribution of some fluid
- $\vec{u} := \nabla\theta$
  Describes its velocity field

Derivation

Let $\psi = \sqrt{\rho} e^{\frac{i\theta}{2}} = \alpha e^{i\beta}$. If we substitute this into the Schrödinger equation, and then split into real and imaginary parts, we get the following:

$$\nabla^2 \alpha - \alpha \nabla \beta \cdot \nabla \beta - \frac{2m}{\hbar^2} V \alpha - \alpha \frac{2m}{\hbar} \frac{\partial \beta}{\partial t} = 0 \tag{1}$$

$$\alpha \nabla^2 \beta + 2 \nabla \alpha \cdot \nabla \beta + \frac{2m}{\hbar} \frac{\partial \alpha}{\partial t} = 0 \tag{2}$$

Derivation (cont.)

The imaginary part, equation 2, when we substitute $\varphi = -\frac{\beta\hbar}{m}$, and noting that $\frac{\partial(\alpha^2)}{\partial t} = 2\alpha\frac{\partial\alpha}{\partial t}$, yields

$$\begin{aligned} \frac{\hbar}{m}\alpha^2\nabla^2\beta + 2\frac{\hbar}{m}\alpha\nabla\alpha\cdot\nabla\beta + \frac{\partial}{\partial t}\alpha^2 &= \alpha^2\nabla^2\varphi + 2\alpha\nabla\alpha\cdot\nabla\varphi + \frac{\partial}{\partial t}\alpha^2 \\ &= \nabla\cdot(\alpha^2\nabla\varphi) + \frac{\partial}{\partial t}\alpha^2 \\ &= 0 \end{aligned}$$

Thus, we have a conservation equation where α^2 is the density of some fluid, and $\nabla\varphi$ is the velocity of the flow.

Derivation (cont.)

The real part, equation 1, under the same substitution, yields

$$\frac{\partial \varphi}{\partial t} + \frac{1}{2}\nabla\varphi \cdot \nabla\varphi - \frac{\hbar^2}{2m^2}\frac{\nabla^2\alpha}{\alpha} + \frac{V}{m} = 0$$

which corresponds to the integral of the Euler equations for irrotational flow. Because $\nabla \times \vec{u} = \nabla \times \nabla\varphi = 0$, taking the gradient yields the familiar Euler equation,

$$\frac{\partial u}{\partial t} + \vec{u} \cdot \nabla u = -\frac{1}{m}\nabla\left(V - \frac{\hbar^2}{2m}\frac{\nabla^2\alpha}{\alpha}\right)$$

Together, the imaginary and real parts of the transformed Schrödinger equation produce the Madelung equations

The Madelung Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \tag{3}$$

$$\frac{D\vec{u}}{Dt} = \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\frac{1}{m} \nabla (Q + V) \tag{4}$$

where

$$Q = -\frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}}$$

is the Bohm potential

Quantum Pressure Tensor

Consider the force due to the Bohm potential,

$$\vec{F}_Q = -\nabla Q = -\frac{m}{\rho} \cdot \vec{p}_Q$$

where

$$\vec{p}_Q = -\frac{\hbar^2}{4} \rho \nabla \otimes \nabla \ln \rho$$

is the quantum pressure tensor

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Madelung Transformation for the Dirac Equations

- The quantum hydrodynamic formulation of Dirac equation and its generalized stochastic and non-linear analogs
  https://arxiv.org/ftp/arxiv/papers/1406/1406.0595.pdf
- Hydrodynamic representation and energy balance for Dirac and Weyl fermions in curved space-times
  https://doi.org/10.1140/epjc/s10052-022-10853-5

Spin and the Pauli Spinor

The Schrödinger equation, with spin, corresponds to spin eigenstates. Given some external electromagnetic vector potential A, we require a wave function factorizable into a a non-spin (Madelung transform) and spin part (χ, Pauli Spinor), which gives an extended Madelung transformation as

$$\psi \equiv \sqrt{\rho} e^{\frac{i\theta}{2}} \chi$$

where the local spin vector $\vec{s} \equiv \chi^* \hat{s} \chi =$ some constant
See https://www.osti.gov/etdeweb/servlets/purl/443237

Quantum Vorticity

Consider time-independent Schrödinger equation in a 3 dimensional Coulomb potential. Analytically, the irrotational assumption falls apart

$$\nabla \times \vec{u} \equiv \begin{bmatrix} 0 \\ 0 \\ \delta(x)\delta(y) \end{bmatrix}$$

Such quantum quasi-irrotational fields promote propagation of vorticity $\omega = \nabla \times \vec{u}$ in time as

$$\frac{\partial \omega}{\partial t} = \nabla \times (\vec{u} \times \omega)$$

Some texts suggest using this term in addition to the Hamilton-Jacobi-esque Madelung equations.

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Smoothed Particle Hydrodynamics

Smoothed particle hydrodynamics (SPH) is a method traditionally used to simulate equations for astrophysics, but has been adapted over the years to be applied to the Navier Stokes and Euler equations for solving fluids

- Automatically adaptive in resolution (domain is unbounded)
- Satisfies conservation condition by construction
- Simple to implement, but slow to compute as the number of particles increases

Smoothed Particle Hydrodynamics (cont.)

SPH leverages a kernel convolution to discretize a field

$$A(\vec{x}) = \int A(\vec{x}')\delta(\vec{x} - \vec{x}')dx'$$

We approximate the Dirac delta function with a Gaussian smoothing kernel, whose integral over space is 1

$$W(\vec{x}; h) = \frac{1}{\pi h^2} \exp\left(-\frac{\|\vec{x}\|^2}{h^2}\right)$$

with smoothing length h such that $\lim_{h\to 0} W = \delta$.
Alternative kernels that have compact support are less computationally expensive, but also less accurate

SPH Field Approximation

We approximate fields by its smoothed average over N particles

$$A(\vec{x}) \approx \langle A(\vec{x}) \rangle = \sum_j \frac{m_j}{\rho_j} A(\vec{x}_j) W(\vec{x} - \vec{x}_j; h) \tag{5}$$

We can approximate gradients and higher order derivatives by shifting the operator to the kernel, whose derivatives are analytically known

Gaussian Kernel

Gaussian Kernel

$$W(\vec{x}; h) = \frac{1}{\pi h^2} \exp\left(-\frac{\|\vec{x}\|^2}{h^2}\right) \tag{6}$$

Gradient of Gaussian Kernel

$$\nabla W(\vec{x}; h) = -\frac{2}{h^2} W(\vec{x}; h)\vec{x} \tag{7}$$

Hessian of Gaussian Kernel

$$\nabla^2 W(\vec{x}; h) = \frac{2}{h^2} W(\vec{x}; h) \left(\frac{2}{h^2}\vec{x} \otimes \vec{x} - I\right) \tag{8}$$

Calculating Density and its Derivatives

We substitute $\rho(\vec{x})$ for $A(\vec{x})$ in equation 5 and find

$$\rho_i = \sum_j m_j W_{ij} \tag{9}$$

where $W_{ij} = W(\vec{x}_i - \vec{x}_j; h)$.
This has first derivatives

$$\nabla \rho_i = \sum_j m_j \nabla W_{ij} \tag{10}$$

and second derivatives

$$\nabla^2 \rho_i = \sum_j m_j \nabla^2 W_{ij} \tag{11}$$

Calculating Pressure Tensor

We choose to discretize the quantum pressure tensor instead of the Bohm potential as it is easier to discretize

$$P_i = \sum_j \frac{m_j}{\rho_j} \frac{1}{4} \left[\frac{1}{\rho_j} \nabla \rho_j \otimes \nabla \rho_j - \nabla^2 \rho_j \right] W_{ij} \tag{12}$$

Updating Particle Positions

Acceleration update:

$$\frac{d\vec{u}_i}{dt} = -\frac{\nabla V}{m} - m\sum_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2}\right)\nabla W_{ij} \tag{13}$$

Velocity update:

$$\vec{u}_i^{n+1} = \vec{u}_i^n + \frac{d\vec{u}_i}{dt}\Delta t \tag{14}$$

Position update:

$$\vec{x}_i^{n+1} = \vec{x}_i^n + \vec{u}_i^{n+1}\Delta t \tag{15}$$

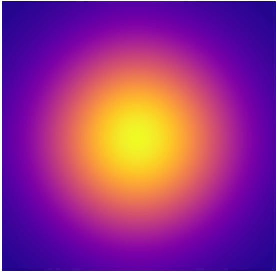
Artificial Dampening for Stationary States

To promote convergence to stationary states faster, we add an artificial dampening term

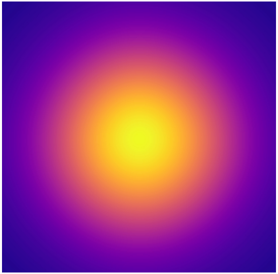
$$\frac{d\vec{u}_i}{dt} = \lambda \vec{u}_i \tag{16}$$

For our tests we choose (somewhat arbitrarily), $\lambda = -0.75$

We initialize particle positions with uniform random distribution, and initialize particle velocities to 0. We choose $\lambda = -0.75$ for the dampening factor, and use $V = \frac{1}{2}\vec{x}^2$.
This has analytical solution $\rho = \frac{1}{\pi}\exp(-\vec{x}^2)$



(a) Computed solution

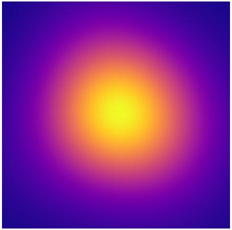


(b) Analytical solution

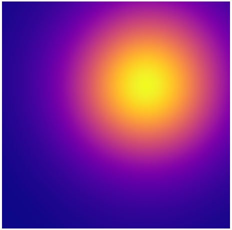
Local Demo

Results: Time Dependent 2D Harmonic Oscillator

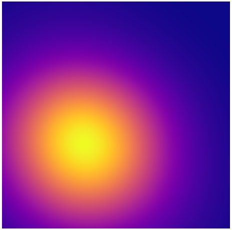
We initialize particle positions to the ground state, and initialize particle velocities to $\vec{u}_i = [1,1]$. We choose $\lambda = 0$ for the dampening factor, and use $V = \frac{1}{2}\vec{x}^2$.
This has analytical solution $\rho = \frac{1}{\pi}\exp(-(\vec{x} - \sin(t))^2)$



(c) Computed t=0s



(d) Computed t=1.5s



(e) Computed t=3s

Local Demo

Thank you!

Any questions?

Check out the code here

- https://github.com/Orikson/Madelung-Equations