Hydrodynamics of the Rotating Spherical Matter Fields and Atomic Structure

İbrahim Mutlay *

Department of Chemical Engineering, Ankara University, 06100 Ankara, Turkey

Abstract

Atomic structure model was proposed as a rotating stratified fluidic matter field with the particles corresponded to solitary waves in the field. Mathematical formulation of the proposed structure was constructed on the model of thermal convection in rotating spherical shells of conducting fluids using magnetohydrodynamic Navier-Stokes Equations. Acceleration term was derived using Coulomb potential. Novel model showed that internal structure of atoms is subjected to complex fluid dynamics.

Classical atom model proposed by Bohr [1] is based on the idea of electrons orbiting around the nucleus and the energy levels of $\Delta E = h\nu$. The model was achieved an excellent success and led to modern chemistry and quantum mechanics. Quantum mechanics revolutionized our views about atomic systems and brought important concepts in scientific knowledge such as the Schrödinger equation [2] for dynamics of particles, wave-particle duality $\Psi(r,t)$ and probability density $\rho := |\Psi(r,t)|^2$. Quantum optics, ultracold fluids, Standard Model, quantum chemistry, nanoscience and other numerous scientific and technological achievements have been obtained using quantum mechanics. However, during the progress, serious problems have arisen especially related with ontological paradoxes [3] and analysis of the many-body systems.

Since the beginning alternative scenarios for quantum phenomena have been suggested trying to overcome the above mentioned difficulties. One of the most important of them, hydrodynamic approach and its applications [4, 5, 6] has given brilliant results in different areas such as density functional theory, quantum transport, superfluids, Bose-Einstein condensation, ultracold fermions, atom optics, BCS superconductivity etc. In this approach which assumes the particles as "quantum fluid" one can easily calculate the physical parameters of the systems containing large number of particles in a superior agreement with the experimental observations. Applicability and success of hydrodynamic viewpoint of quantum mechanics are valid for wide ranging scales from predicting the properties of bulk materials to molecular structures, even to chemical bonds. Recently, in two different studies, researchers modeled individual chemical bonds using electron flux [7, 8]. In [7] Okuyama and Takatsuka theoretically pictured the "electron

^{*}E-mail: ibrahimmutlay@gmail.com

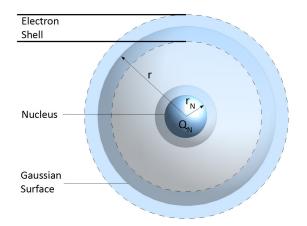


Figure 1: Stratified spherical matter field as proposed atomic structure model (not to scale). Q_N is the total charge of nucleus; Gaussian surface is spherically symmetric and concentric with the nucleus.

flow" around sodium and chlorine nuclei while Barth et al. [8] used H_2^+ as a model system with a similar technique and acquired quite promising results.

Hyrodynamic interpretation of quantum mechanics mathematically stems from the Madelung transformation $\psi = \sqrt{\rho} \exp[i\phi]$ in the time-dependent Schrödinger Equation [4]:

$$i\hbar\frac{\partial}{\partial t}\psi(r,t) = -\frac{\hbar^2}{2m}\,\nabla^2\,\psi(r,t) + V(r,t)\psi(r,t) \tag{1}$$

Denoting $\psi(r,t)$ as wavefunction, m as particle mass, $\hbar = \frac{h}{2\pi}$ with Planck constant h and V(r,t) as external potential. After some mathematical manipulation, taking velocity potential field as $\mathbf{u}(r,t) = \frac{\hbar}{m} \nabla \phi(r,t)$ and separating the real and imaginary parts of the resulting equation we obtain [4, 9, 10]:

$$\frac{\partial}{\partial t}\rho(r,t) = -\nabla \cdot \rho(r,t)\mathbf{u}(r,t)$$
(2)

$$\frac{\partial}{\partial t}\mathbf{u}(r,t) + \mathbf{u}(r,t) \cdot \nabla \mathbf{u}(r,t) = -\nabla \mu_Q - \frac{1}{m}\nabla V(r,t)$$
(3)

It is obvious from the above equations that the time-dependent Schrödinger Equation is equivalent to Euler equations of fluid dynamics. Connection of these equations to quantum mechanics is through the "quantum chemical potential" term: $\mu_Q = -\frac{\hbar^2}{2m}\frac{1}{\rho}\left(\nabla^2\rho - \frac{1}{2\rho}(\nabla\rho)^2\right)$. ρ is also not classical density but it is the probability density $\rho = |\psi(r,t)|^2$ in a phase space.

We begin to construct the mathematical formulation of our model by presenting some important assumptions. Now, let us suppose that all the particles are the excitations (solitary waves) in a matter field. Main proof for this assumption can be found in Unruh's seminal work [11] revealing that the field equations of phonons in a nonhomogeneous fluidic matter correspond to the relativistic field in a 4D curved space-time [11, 12]. Such a matter field would be defined by density, temperature and composition $\Psi := \mathcal{F}(\rho, T, \mathbf{X})$. Composition is relevant to the flavor concept of particle physics and probability density of quantum mechanics, in contrast to the standard definition, is exactly the classical matter density given in the field definition.

Seeing above theorems, we can build the mathematical equations governing the dynamics of our model. We will assume that the fermionic matter field surrounding the nucleus is a rapidly-rotating stratified spherical shell of electrically conducting Boussinesq fluid (see Fig. 1) moved under the magnetohyrodynamic and thermally convective actions i.e. Lorentz, buoyancy and Coriolis forces. Additionally, thermophysical and magnetic properties of the fluidic matter will be constant [13].

In the light of this scheme, combining magnetohydrodynamic Navier-Stokes equations, Maxwell's equations and the heat equation we arrive at following system of differential equations governing our model:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + 2\Omega \mathbf{k} \times \mathbf{u} = -\frac{1}{\rho} \nabla p + \alpha \Theta a_C \mathbf{r} + \frac{1}{\rho \mu} (\nabla \times \mathbf{B}) \times \mathbf{B} + \nu \nabla^2 \mathbf{u}$$
(4)

$$\frac{\partial \Theta}{\partial t} + \mathbf{u} \cdot \nabla \Theta + \mathbf{u} \cdot \nabla T_s = \kappa \nabla^2 \Theta \tag{5}$$

$$\frac{\partial}{\partial t}\mathbf{B} + \mathbf{u} \cdot \nabla \mathbf{B} = \mathbf{B} \cdot \nabla \mathbf{u} + \lambda \nabla^2 \mathbf{B}$$
(6)

with the condition of incompressibility : $\nabla \cdot \mathbf{u} = 0$ (7)

where **u** is velocity field, Ω is angular velocity, **k** is rotation unit vector, ρ is density, p is pressure, α is thermal expansion coefficient, Θ is temperature field, a_C is Coulomb acceleration, **r** is position vector, μ is magnetic permeability, **B** is magnetic field, ν is kinematic viscosity, T_s is steady temperature, κ is thermal diffusivity and λ is magnetic diffusivity.

Rewriting the equations of (4-6) via nondimensionalization would be convenient since in computation, experimental testing or other analysis studies scaled equations is extremely functional. We define required dimensionless parameters in such a manner that $D = r_0 - r_i$ is length, $\frac{D^2}{\nu}$ is time, $\frac{\nu}{D}$ is velocity, $\rho\nu\Omega$ is pressure and $\Delta\Theta$ is average gradient of temperature T_s [14]. In fluid dynamics, the Rayleigh, Ekman, Prandtl and magnetic Prandtl dimensionless numbers are highly useful for the problems especially the ones resembling discussed here. Denoting the numbers respectively as Ra, E, PrPm:

$$Ra = \frac{\alpha a_C \Delta \Theta D^3}{\kappa \nu} \tag{8}$$

$$E = \frac{\nu}{\Omega D^2} \tag{9}$$

$$Pr = \frac{\nu}{\kappa} \tag{10}$$

$$Pm = \frac{\nu}{\lambda} \tag{11}$$

Derivation of the nondimensional form of the equations (4-6) can be accomplished by applying the dimensionless numbers. The Rayleigh number is described as the ratio of buoyancy force to viscous dissipation; the Ekman number is the ratio of the viscous force to Coriolis force; the Prandtl number corresponds to the ratio of momentum diffusivity to thermal diffusivity while magnetic Prandtl number is the ratio of momentum diffusivity (viscosity) and magnetic diffusivity.

Fermionic fluid surrounding the atomic coordinates is affected by Coulomb potential originating from nucleus. This effect is expressed in Coulomb acceleration, a_C term of equation (4). a_C can be derived in a straightforward way using Gauss's law. Let E_r be electric field acting on Gaussian surface of Figure 1:

$$E_r = \frac{1}{4\pi\epsilon_0} \frac{Q_N}{r^2} = \frac{m_e a_C}{q}$$

Where Q_N is the total charge of nucleus, ϵ_0 is vacuum permittivity (electric constant), r is the radius of the sphere enveloped by Gaussian surface, q is the total charge of fermionic field at Gaussian surface and m_e is the mean field mass of fermionic matter field. Accordingly Coulomb acceleration would be:

$$a_C = \frac{1}{4\pi\epsilon_0} \frac{qQ_N}{m_e r^2} \tag{12}$$

Developing solutions for equations of (4-6) is a quite tough problem. Computational techniques are available but they all consist of source consuming procedures. Instead of that we can assess them in simple terms. Let us deal with a system with no rotation $\Omega = 0$, no magnetic field $\mathbf{B} = 0$ and inviscid flow $\nu = 0$. These assumptions lead equation (4) to the form given below:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \alpha \Theta a_C \mathbf{r}$$
(13)

In comparison with equation (3) we can see that there is an evident correspondence between quantum hydrodynamics and proposed model. Moreover, it is apparent that quantum chemical potential is related to an intrinsic pressure dominating in quantum fluid: $\frac{1}{\rho}\nabla p := \nabla \mu_Q(\rho)$. Another important observation is $\alpha \Theta a_C \mathbf{r} := -\frac{1}{m}\nabla V(r,t)$ correspondence which gives clues about the physical nature of the external potential of equation (3). It seems that in the motion of quantum fluidic matter field thermal convective processes play a crucial role.

We suggested and discussed a novel atomic structure model described as a stratified and spherically symmetric fermionic fluidic matter field around a condensed nucleus. Relations between Madelung's equations (Eqs. 2-3) and our model (Eqs. 4-6) pointed out the interesting nature of quantum hydrodynamics. Numerical analysis could not be executed due to complexity of the problem but computational fluid dynamics of rotating spherical systems is a highly studied topic especially in the field of geophysics and it is possible to employ the results available in this literature [13, 14, 15]. Al-Shamali et al. [14] obtained a flow pattern with localized modes in equator of the spherical system for Pr = 1, $Ra = 0 - 13.2 \times 10^{-5}$, $E = 3 \times 10^{-4}$ and $\mathbf{B} = 0$. Such a localized flow structure should be involved in the origins of quantum mechanical phenomena for atoms. However toward a more deeper understanding, further computational analysis of our model must be carried out. Finally, we can say that proposed atomic model is more realistic and more consistent with the many-body condensed matter systems such as solid state structures. Besides, in the attempts of extending quantum mechanics to cosmology, our model could be beneficial. Recently there is a hugely growing interest to figure out the gravitational problems using cosmological fluid dynamics especially in terms of AdS/CFT correspondence [16]. It is clear that hydrodynamic formulation of quantum mechanics will be more compatible with cosmology.

References

- Niels Bohr, "On the constitution of atoms and molecules", Philosophical Magazine Series 6, Volume 26, Issue 151 July 1913, pages 1 - 25.
- Schrödinger, E., "An Undulatory Theory of the Mechanics of Atoms and Molecules". Physical Review 28 (6): 1049–1070, 1926.
- [3] Einstein, A., Podolsky, B., Rosen, N., "Can quantum-mechanical description of physical reality be considered complete?", Physical Review 47: 777-780, 1935.
- [4] Madelung, E., "Quantentheorie in hydrodynamischer Form". Z. Phys. 40: 322–326, 1927.
- [5] P. Hohenberg, W. Kohn, "Inhomogenous electron gas", Phys. Rev. 136, B864, 1964.
- [6] Radomir Slavchov and Roumen Tsekov, "Quantum hydrodynamics of electron gases", J. Chem. Phys. 132, 084505, 2010.
- [7] Michihiro Okuyama, Kazuo Takatsuka, Electron flux in molecules induced by nuclear motion, Chemical Physics Letters 476, 109–115, 2009.
- [8] Ingo Barth, Hans-Christian Hege, Hiroshi Ikeda, Anatole Kenfack, Michael Koppitz, Jörn Manz, Falko Marquardt, Guennaddi K. Paramonov, Concerted quantum effects of electronic and nuclear fluxes in molecules, Chemical Physics Letters 481, 118–123, 2009.
- [9] L.A. Turski, "Dissipative Quantum Hydrodynamics", Acta Physica Polonica B, No:7, Vol. 26, 1995.

- [10] A. Visinescu, D. Grecu, R. Fedele, S. De Nicola, "Madelung Fluid Description of the Generalized Derivative Nonlinear Schrodinger Equation: Special Solutions and Their Stability", Theoretical and Mathematical Physics, 160(1): 1066–1074, 2009.
- [11] W. G. Unruh, "Experimental Black-Hole Evaporation?", Phys. Rev. Lett. 46, 1351–1353, 1981.
- [12] Jean Macher and Renaud Parentani, "Black/white hole radiation from dispersive theories", Phys. Rev. D 79, 124008, 2009.
- [13] Keke Zhang, Gerald Schubert, "Magnetohydrodynamics in Rapidly Rotating Spherical Systems", Annu. Rev. Fluid Mech. 2000. 32:409–443
- [14] F.M. Al-Shamali, M.H. Heimpel, J.M. Aurnou, "Varying the Spherical Shell Geometry in Rotating Thermal Convection", Geophysical and Astrophysical Fluid Dynamics Vol. 98, No. 2, April 2004, pp. 153–169.
- [15] P D Mininni, D C Montgomery, L Turner, "Hydrodynamic and magnetohydrodynamic computations inside a rotating sphere", New Journal of Physics 9, 303, 2007.
- [16] Mukund Rangamani, "Gravity and hydrodynamics: lectures on the fluid-gravity correspondence", Class. Quantum Grav. 26, 224003, 48pp, 2009.