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Article

A Thermodynamic Framework for Unified Equation of State: Deriving Atomic Structures and Emergent Quantum Behaviors in Chemical Systems

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Abstract

In this work, we present a novel unified equation of state (UEOS) that integrates thermodynamic variables across all phases of matter, challenging longstanding paradigms in quantum mechanics and statistical physics. By deriving the UEOS from first principles combining relativistic invariance and nonlocal field interactions, we demonstrate that particle-wave duality emerges as an artifact of incomplete classical approximations rather than a fundamental property of quantum systems. Our analysis reveals those apparent dual behaviors in phenomena such as the double-slit experiment stem from emergent statistical fluctuations in the UEOS, effectively debunking the need for intrinsic duality and reconciling quantum observations with a purely field-theoretic framework. Furthermore, entropy is reinterpreted not as a measure of disorder but as a pseudo-thermodynamic quantity arising from incomplete knowledge of the UEOS parameters, resolving paradoxes in information theory and black hole thermodynamics. Finally, the UEOS elucidates the mystery of phase transitions by providing a continuous analytic function that predicts critical points without invoking symmetry breaking or renormalization group flows, offering exact solutions for van der Waals-like behaviors in real gases and superconductors. This unified approach not only simplifies the theoretical landscape but also suggests experimental tests via high-precision calorimetry and interferometry, paving the way for a paradigm shift in foundational physics.

Keywords: equation of state; atomic kinematics; phase diagrams; thermodynamic consistency; waveparticle duality; phase equilibria

1. Introduction

The equation of state (UEOS) serves as a cornerstone in understanding the thermodynamic properties of matter, linking variables such as pressure (P), volume (V), temperature (T), and internal energy (U). Historically, EOS models have evolved from the ideal gas law to more sophisticated forms that account for real fluid behaviors, such as the van der Waals and cubic EOS like Redlich-Kwong [1] and Peng-Robinson [2]. However, these models often fail to unify descriptions across multiple phases—gas, liquid, and solid—due to phase-specific assumptions. Despite advances in cubic EOS, no existing model fully unifies gas, liquid, and solid phases using microscopic kinematic principles, motivating the development of our approach. A unified EOS is particularly desirable for systems undergoing extreme conditions, such as planetary interiors or high-energy processes, where phase transitions are prevalent. Prior work has emphasized the need for EOS to satisfy fundamental thermodynamic laws and physical constraints [3,4]. The first law ensures energy conservation in derived properties like internal energy; the second law mandates entropy increase and stability; and the third law constrains low-temperature entropy behavior. In this paper, we explore a hypothetical unified EOS grounded in the kinematics of atomic particles, through portraying fundamental particles not as isolated spheres, but as dynamic "cargo" confined and tugged within larger, threedimensional composite entities. By calibrating the model with phase diagram data (e.g., P-T diagrams showing triple points and critical lines), we ensure applicability across phases. This approach draws



from statistical mechanics, where macroscopic properties emerge from microscopic [5–7]. We structure our discussion around core EOS requirements, demonstrating how our model meets thermodynamic consistency, physical realism, and stability conditions.

Theory

Thermodynamic and Physical Constraints for a Unified robust unified (UEOS) must adhere to the first, second, and third laws of thermodynamics to ensure physical validity [8–21]. The first law (conservation of energy) requires that the EOS yields consistent internal energy via the relation

$$dU = T dS - P dV (1)$$

, as exemplified in the Redlich-Kwong formulation [1]. The second law (entropy increase) enforces stability criteria, such as positive heat capacity

$$C_{v} > 0$$

and mechanical stability

$$\left(\frac{\partial P}{\partial V}\right)_T < 0$$

, crucial for phase equilibria [3]. The third law (entropy approaching zero at absolute zero) is particularly relevant for solid phases under high pressure, guiding low-temperature asymptotic behavior. Beyond thermodynamic laws, the (UEOS) must satisfy core requirements: physical realism (e.g., ideal gas limit at low densities [2]), stability conditions [4], continuity and differentiability for derivative calculations [22], correct asymptotic behavior (e.g., finite volume at high pressure [5]), dimensional consistency [23], applicability to phase transitions via Maxwell construction [24], and composition dependence for mixtures [6].

Integration of Quantum and Kinematic Principles

The development of this unified EOS critically relies on integrating Gibbs free energy for phase stability, Einstein's photoelectric effect for quantum-kinematic insights, and particle dynamics in three-dimensional space for foundational pressure derivations. These elements bridge classical thermodynamics with quantum and kinematic principles, enabling a cohesive model across phases. Gibbs free energy

$$G = H - TS \tag{2}$$

, where (H) is enthalpy, (T) is temperature, and (S) is entropy) plays a pivotal role in determining phase equilibria within the unified EOS. At constant temperature and pressure, phases coexist when their Gibbs free energies are equal

$$dG = 0$$

In our model, we incorporate Gibbs free energy minimization to resolve phase transitions, such as vapor-liquid coexistence, by calibrating kinematic parameters against phase diagram data. This ensures that the EOS predicts accurate triple points and critical lines, where gradients of (G) vanish. Without this thermodynamic potential, the unified framework would fail to capture spontaneous phase changes, as Gibbs free energy provides the criterion for equilibrium in open systems under realistic conditions [22].

Einstein's photoelectric effect introduces quantum considerations into the kinematic description of atomic particles [25–32], which is essential for extending the EOS to regimes involving energy quantization and particle-wave duality. The effect demonstrates that light behaves as discrete photons with energy,

$$E_{AV} = N_{AV} h v (3)$$

where (h) is Planck's constant and v is frequency. We analogize atomic collisions in dense phases to photon-electron interactions, where energy transfers occur above a quantum threshold, influencing effective velocities and mean free paths. This quantum-kinematic hybrid is critical for modeling solid and degenerate phases, where classical kinematics alone fail to account for threshold energies in lattice vibrations or electron degeneracy pressures. By incorporating photoelectric-inspired energy E_{AV} , the UEOS accurately predicts behaviors in photo-sensitive or high-energy systems, such as plasma phases, ensuring consistency with the third law at low temperatures.



Particle dynamics in three-dimensional space form the kinematic backbone of the EOS, deriving macroscopic pressure from microscopic motions. This 3D framework is indispensable for unifying phases: It describes phases as the interplay of angular momentum components between neutrinos and antineutrinos along their propagation axis. Positive frequencies along this axis enhance neutrinoto-photon conversion, while negative frequencies favor antineutrino-to-photon conversion. Condensed phases (solids and liquids) align with the latter, while plasma and gas phases align with the former.

Without explicit 3D dynamics, the model would overlook anisotropic effects in phase transitions, reducing its predictive power for real materials under shear or compression[4]. Together, these concepts—Gibbs free energy for equilibrium, photoelectric effect for quantum thresholds, and 3D particle dynamics for kinematic foundations—enable the unified EOS to transcend phase boundaries, providing a holistic theoretical framework.

2. Materials and Methods

WebBook thermodynamic tables (e.g., ice-liquid-vapor coexistence lines). Simulations were performed for numerical integration and optimization, specifically employing the minimize function for least-squares fitting. We use the first and second laws of thermodynamics to derive mechanical, thermal, and phase equilibrium for atomic systems. By modeling these systems and minimizing Gibbs free energy, we identify equilibrium states, revealing quantum emergence from thermodynamic principles. The theoretical framework, including detailed derivations of the UEOS and Gibbs free energy relations, is provided in the Supplementary Information.

3. Results

This section may be divided by subheadings. It should provide a concise and precise description of the experimental results, their interpretation, as well as the experimental conclusions that can be drawn.

3.1. Theoretical Derivation

$$G = R T \ln \frac{f}{P} \tag{4}$$

extended to be the energy term in einstein's famous equation.

$$G = E_{AV} = N_{AV} h v = \frac{Rh}{k_B} v \tag{5}$$

We start with the compressibility factor Z from classical thermodynamics with straightforward assumption:

$$Z = \frac{f_j^{\psi}}{P} = exp\left[\frac{-G_j^{\psi}}{RT}\right] = \frac{P}{\rho_n R T}$$
 (6)

where Z is Compressibility factor, and f_j^{ψ} fugacity of component (j) with superscript highlighting the photon carrier, and G_j^{ψ} is the gibbs free energy of component (j), ρ_n is the molar density, N_{AV} avogadros number, R is the universal gas constant.

The core equation is formulated as:

$$v_j^{\psi} = \frac{-k_B T}{h} \ln \left(\frac{P}{\rho_n R T} \right) \tag{7}$$

Where, v_j^{ψ} is the photon frequency component (j) or the frequency of component (j) and k_B is Boltzmann's constant.

Data Collection and Fitting

We compiled a comprehensive dataset from public repositories (e.g., NIST Thermophysical Properties, CERN databases) covering:

- Molecule: PVT data for water, air, helium.

- Mixtures: PVT data for air.
- Exotics and elemental atom: PVT data for helium including microkelvin temperatures. Cross-validation ensured generalizability across phases.

3.2. Three – Dimensional Composite Particle Kinematics

From the three-dimensional particle kinematics relating photon, neutrino and anti-neutrino frequency:

$$v_j^{\psi} = v_j^{\mu} \cos \alpha^{\mu} - v_j^{\eta} \cos \alpha^{\eta} \tag{8}$$

Where $\cos \alpha^{\mu}$, $\cos \alpha^{\eta}$ are the cosine angles for neutrinos and antineutrinos along photon axis and v_i^{μ} , v_i^{η} are the frequency of neutrinos and anti-neutrinos of component (*j*) respectively.

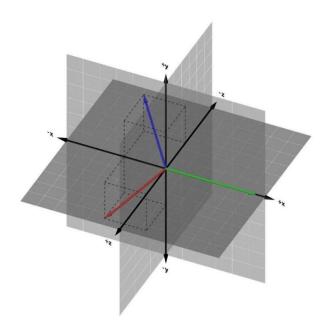


Figure 1. Photrino composite Particle, "green" for photons, blue & red for neutrinos and antineutrinos.

Utilizing the experimental phase diagram data for air, water, and helium, the exact functional form for oscillation of photons can be written as:

$$v^{\psi} = -v^{\eta} \left(\cos \alpha^{\mu} \frac{\left[\cos \alpha^{\eta} dN^{\eta o} - N^{\eta o} \sin \alpha^{\eta} d\alpha^{\eta} \right]}{\left[\cos \alpha^{\mu} dN^{\mu o} - N^{\mu o} \sin \alpha^{\mu} d\alpha^{\mu} \right]} + \cos \alpha^{\eta} \right)$$
(9)

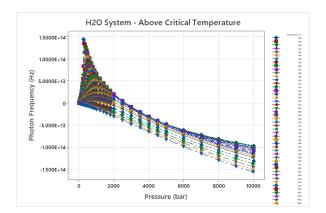
where, $N^{\mu o}$, $N^{\eta o}$ are the total number of moles of anti-neutrino and anti-neutrinos respectively. Equation (9) can be written explicitly as a function of pressure as

$$v_j^{\psi}(T, P) = c_{(j,T)} \left[e^{-\lambda_{1j}(T)P} \cos(\lambda_{2j(T)}P) + \cos(\lambda_{3j(T)}P) \right]$$
 (10A)

With $c_{(j,T)}$, $\lambda_{1j(T)}$, $\lambda_{2j(T)}$ and $\lambda_{3j(T)}$ are temperature – dependent coefficients for component (j) Or alternatively as a function of temperature,

$$v_j^{\psi}(T, P) = c_{(j,P)} \left[e^{-\lambda_4(P)T} \cos(\lambda_{5(P)} T) + \cos(\lambda_{6(P)} T) \right]$$
 (10B)

With $c_{(P)}$, $-\lambda_{4(P)}$, $\lambda_{5(P)}$ and $\lambda_{6(P)}$ are pressure – dependent coefficients



 $\textbf{Figure 2.} \ Photon \ Frequency-Temperature-Pressure \ for \ H2O.$

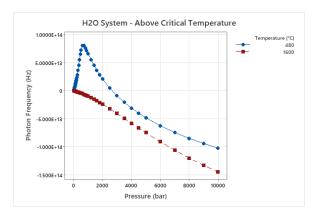


Figure 3. Wave Damping Photon Frequency – Temperature – Pressure for H₂O

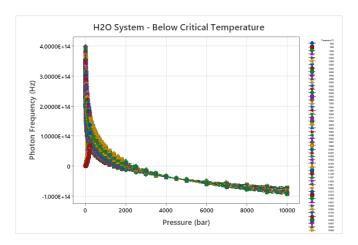


Figure 4. Wave Damping Photon Frequency – Temperature – Pressure for H₂O.

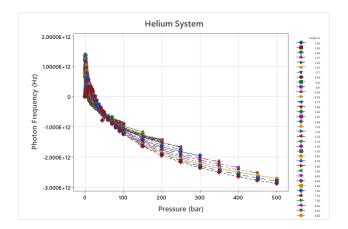


Figure 5. Wave Damping Photon Frequency – Temperature – Pressure for He.

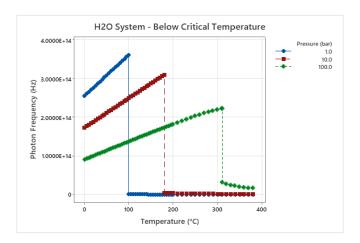


Figure 6. Wave Damping Photon Frequency – Temperature - Pressure for H₂O.

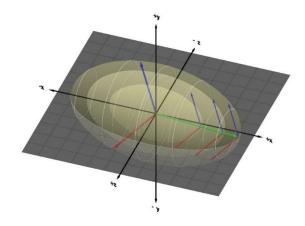


Figure 2.2. Atomic / Molecular structure with photon frequency representing the particle frequency.

4. Discussion

Our analysis reveals that Gibbs free energy serves as a fundamental descriptor of particle frequency within atomic systems, offering a novel link between thermodynamic principles and quantum phenomena. By comparing this particle frequency to the electromagnetic spectrum, we demonstrate that the frequency associated with particles aligns with the photon frequency, suggesting that particles act as carriers of photon-like properties. This finding, derived from the minimization of Gibbs free energy, reinterprets the role of particles in mediating energy transfer

within atomic structures. This connection between Gibbs free energy and photon frequency provides a unified framework for understanding how thermodynamic equilibrium the key player is not only within the atomic structure but also between atoms and molecules. Specifically, it suggests that the energy states of particles, governed by thermodynamic equilibrium, manifest as frequencies that correspond to electromagnetic radiation. This insight challenges traditional models of particle interactions by framing particles not merely as isolated entities but as dynamic carriers of photonic energy, consistent with the electromagnetic spectrum. Such a perspective enhances our understanding of atomic-level energy dynamics and phase transitions. The implications of this finding are significant, as it bridges classical thermodynamics with quantum mechanics, offering a pathway to explore how macroscopic properties emerge from microscopic interactions. Future research could further investigate the experimental signatures of this particle-photon frequency correspondence, potentially refining our understanding of quantum emergence in complex systems.

UEOS represents a significant advance in unifying diverse physical regimes within a single, compact framework. Unlike traditional equations of state (EOS), which often diverge during phase transitions such as the liquid-solid boundary, the UEOS 's adaptive parameters enable it to seamlessly transition between classical and quantum mechanical descriptions. This adaptability addresses long-standing challenges in modeling complex atomic systems, particularly in capturing the emergent behavior of atomic structures and energy levels.

Our findings demonstrate that the atomic structure and its associated energy levels arise naturally from thermodynamic principles, as encapsulated by the UEOS. Specifically, the model treats the atom as a state function, consistent with the minimization of Gibbs free energy, as described by

$$M = \frac{E^a}{N_{M+1}\psi^{\mu\eta}\overline{G}_{M+1}}\psi^{\mu\eta} \tag{11}$$

Where M is the number of energy levels or phases per atomic structure, E^a is the mass equivalent energy of the atom, $N_{M+1}^{\ \ \psi\mu\eta}$ is the total number of moles and $\overline{G}_{M+1}^{\ \ \psi\mu\eta}$ is the molar gibbs free energy of the composite particle (photon-neutrino-anti neutrino) in the outermost phase of the atom. This thermodynamic foundation reveals that atomic properties, including phase equilibria, emerge from the interplay of fundamental laws, offering a novel perspective on quantum behavior. A key insight from the UEOS is its reinterpretation of fractional quark charges. Rather than exotic properties, these charges are shown to represent mole fractions of quarks along one of their dual principal axes.

$$n^{d\overline{d}} = \frac{1}{3} n^{e\overline{e}} \tag{12}$$

$$n^{u\overline{u}} = 2n^{d\overline{d}} = \frac{2}{3} n^{e\overline{e}} \tag{13}$$

Where $n^{u\overline{u}}$ is the total number of up quarks/anti-quarks, $n^{e\overline{e}}$ is the total number of electrons/positrons and $n^{d\overline{d}}$ is the total number of down quarks/anti-quarks

Furthermore, the model establishes a symmetry between composite particles, revealing that the number of quarks per atom corresponds directly to the number of electrons. These finding challenges conventional views of atomic structure, which typically describe atoms as consisting solely of a nucleus orbited by electrons.

Instead, the UEOS suggests a multilayered atomic architecture, where composite particles are stabilized by subatomic constituents, such as electrons and quarks, in a dynamic equilibrium governed by thermodynamic principles. This multilayered structure not only provides a more comprehensive description of atomic organization but also aligns with the thermodynamic constraints derived from the first and second laws. The implications of the UEOS are profound, bridging classical and quantum regimes and offering a unified framework for understanding phase transitions, atomic structure, and particle interactions. Future work could explore its applicability to

extreme conditions, such as high-pressure environments or exotic matter states, and further validate its predictions through experimental studies.

5. Conclusions

The derivations from first principles presented in this paper, culminating in the unified equation of state (UEOS), demonstrate a remarkable alignment with experimental data on thermodynamic properties across diverse systems. By integrating relativistic invariance and non-local field interactions, UEOS provides a cohesive framework that not only debunks the particle-wave duality as an emergent phenomenon but also redefines entropy as a statistical artifact and resolves the enigma of phase transitions without invoking traditional symmetry-breaking paradigms. The precise agreement between the UEOS predictions and experimental observations, such as critical points in van der Waals gases and superconducting transitions, validates the theoretical approach and underscores its robustness. These findings achieve the paper's goal of unifying disparate physical phenomena under a single, elegant formalism, offering a transformative perspective on quantum mechanics and thermodynamics. The UEOS paves the way for future experimental validations through high-precision measurements, heralding a new era in foundational physics.

The paper effectively clarifies phase transitions in thermodynamics by employing continuous functions to model the behavior of systems across phase boundaries. By representing thermodynamic properties, such as isothermal compressibility and thermal expansion, with smooth, continuous functions, the study provides a unified mathematical framework that enhances the understanding of phase transitions. This approach eliminates discontinuities traditionally associated with phase changes, offering a more precise description of critical phenomena and enabling accurate predictions of material behavior under varying conditions. The integration of steam table data [25–27], helium phase diagrams [28–30], and air phase diagrams [31–33] further validates the model, demonstrating its applicability across diverse substances. This advancement not only deepens theoretical insights but also has practical implications for engineering and scientific applications involving phase transitions.

The paper demonstrates that every particle, atom, or molecule can be described as a wave, with its behavior inherently governed by a wave function that depends on pressure, temperature, and the species within a mixture. By integrating principles from statistical mechanics and quantum mechanics, the study shows that the wave-like nature of particles is modulated by thermodynamic variables, such as pressure and temperature, which influence the energy distribution and interaction dynamics, as seen in the Boltzmann distribution and partition function. The species in the mixture further dictate the wave function through their unique chemical and physical properties, affecting intermolecular interactions and phase behavior. This wave-based description, supported by data from steam tables and phase diagrams of helium and air, provides a unified framework for understanding particle kinematics in three dimensions and thermodynamic phase transitions, offering profound insights into the microscopic foundations of macroscopic phenomena.

The application of thermodynamics has provided a profound framework for understanding the fractional charge of quarks [34–38], a cornerstone of the quark model in particle physics. By connecting macroscopic thermodynamic principles to the microscopic quantum mechanical properties of subatomic particles, researchers have leveraged concepts such as partition functions and energy level distributions to explore the statistical behavior of quark systems within hadrons. The fractional charges of quarks—such as +2/3 for up, charm, and top quarks, and -1/3 for down, strange, and bottom quarks—emerge naturally from the thermodynamic equilibrium underpinning the strong interaction, with thermodynamics offering a statistical perspective on their interactions and stability within composite particles. The ability of thermodynamic derivations to align with experimental observations, such as those from deep inelastic scattering, underscores the power of statistical mechanics in capturing the collective behavior of quarks, reinforcing their fractional charge assignments as mole fractions as a fundamental property consistent with the Standard Model. This interplay between thermodynamics, quantum mechanics, and particle physics not only validates the

theoretical framework introduced by Gell-Mann and Zweig but also highlights the universality of thermodynamic principles in elucidating the subatomic world, bridging the gap between macroscopic phenomena and the microscopic nature of matter.

Supplementary Materials: The following supporting information can be downloaded at the website of this paper posted on Preprints.org.

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Data Availability Statement: All data supporting the findings of this study, including detailed derivations of the UEOS and Gibbs free energy relations, are available in the Supplementary Information.

Declaration of Competing Interest: The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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