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Python-Based Visualization of Fermi-Dirac and Bose-Einstein Distributions in Three-Dimensional Ideal Quantum Gases

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ABSTRACT

Quantum statistics describe the behavior of indistinguishable particles through the Fermi–Dirac (FD) and Bose–Einstein (BE) distributions. This study compares both distributions directly to emphasize their fundamental statistical differences. A Python-based computational model was developed to visualize the contrasting behaviors of FD and BE distributions in a unified 3D representation. The simulation uses NumPy and Matplotlib with an energy interval of 0.01–1.00 eV, temperatures ranging from 100 K to 600 K, and a chemical potential of $\mu = 0.5$ eV. The results show that the FD distribution forms a sharp profile near the Fermi energy and becomes step-like at low temperatures, while the BE distribution rises sharply as the chemical potential is approached, reflecting the characteristic mathematical divergence of Bose–Einstein statistics rather than indicating actual Bose–Einstein condensation. As temperature increases, the differences between the Fermi–Dirac and Bose–Einstein distributions become less pronounced, consistent with the expected high-temperature limit. The model yields an average relative deviation below 0.5%, confirming numerical stability and accuracy. This work provides an open-source Python framework for the visualization and comparative analysis of ideal quantum statistical distributions, intended primarily for educational and computational purposes rather than for predicting new physical phenomena.

Keywords: Bose–Einstein Distribution, Computational Simulation, Fermi–Dirac Distribution, Python, Quantum Statistics

ABSTRAK

Statistik kuantum menggambarkan perilaku partikel yang tidak dapat dibedakan melalui distribusi Fermi–Dirac (FD) dan Bose–Einstein (BE). Studi ini membandingkan kedua distribusi secara langsung untuk menekankan perbedaan statistik mendasar mereka. Sebuah model komputasi berbasis Python dikembangkan untuk memvisualisasikan perilaku yang kontras dari distribusi FD dan BE dalam representasi 3D yang terpadu. Simulasi menggunakan NumPy dan Matplotlib dengan interval energi 0,01–1.00 eV, suhu 100–600 K, dan potensial kimia $\mu = 0{,}5$ eV. Hasilnya menunjukkan bahwa distribusi FD membentuk profil tajam di dekat energi Fermi dan menjadi seperti tangga pada suhu rendah, sementara distribusi BE naik tajam mendekati potensial kimia, mencerminkan divergensi matematis khas distribusi Bose–Einstein, bukan menunjukkan kondensasi Bose–Einstein yang sesungguhnya. Seiring dengan meningkatnya suhu, perbedaan antara distribusi Fermi-Dirac dan Bose-Einstein menjadi semakin tidak mencolok, selaras dengan kondisi batas suhu tinggi yang diharapkan. Model ini menghasilkan deviasi relatif rata-rata di bawah 0,5%, yang mengonfirmasi stabilitas dan akurasi numeriknya. Penelitian ini menyajikan kerangka kerja Python sumber terbuka untuk visualisasi dan analisis komparatif distribusi statistik kuantum ideal, yang utamanya ditujukan untuk tujuan pendidikan dan komputasi, bukan untuk memprediksi fenomena fisika baru.

Kata kunci: Distribusi Bose-Einstein, Distribusi Fermi-Dirac, Python, Simulasi Komputasi, Statistik Kuantum

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1. Introduction

Quantum statistics offers a basic framework to understand the behaviour of identical particle systems, be it fermionic (e.g. electrons) or bosonic (e.g. photons and ultracold atoms). With this formalism, the relationship between microscopic properties of particle and macroscopic parameters for system such as energy, temperature and pressure can be consistently discussed. This framework is expressed through two main distributions, Fermi–Dirac (FD) distribution for fermions and Bose–Einstein (BE) distribution for bosons. These distributions play an important role in quantum statistical physics and are widely used to describe various quantum phenomena, including superconductivity, superfluidity, and Bose–Einstein condensation under appropriate physical conditions [1]. Recent numerical studies have also investigated quantum statistical systems involving bosonic and fermionic particles, particularly in describing Bose–Einstein condensation and Fermi–Dirac relaxation phenomena through deterministic computational approaches [2].

The FD distribution describes particles that follow the Pauli exclusion principle, which prohibits two fermions to be simultaneously in the same quantum state. In contrast, the BE distribution describes bosons, which may occupy the same quantum state simultaneously. Under appropriate physical conditions, such behavior can lead to Bose–Einstein condensation at sufficiently low temperatures [3], [4]. Visualizing both distributions simultaneously provides an intuitive means of illustrating the fundamental statistical differences between fermions and bosons. In addition, Python-based computational toolkits such as QuSpin provide numerical support for modeling fermionic many-body systems.

Computational simulations provide a bridge between analytical theory and complex quantum phenomena, and play an important role in contemporary physics research, as well as its instruction. Because of its efficient numerical capabilities, extensive scientific libraries, and data-driven visualization tools, Python has become one of the most widely used programming languages for scientific computing. Using this approach, the BE and FD distributions can be studied to illustrate how energy, temperature, and chemical potential influence particle occupation, making it a valuable tool for teaching quantum statistics. Using this method, BE and FD distributions can be studied together to see how energy, temperature, and chemical potential influence the probability of particle occupancy and it is a good way in teaching [5], [6].

Several previous studies have employed Python to support various applications in quantum physics and computational science. Caruso et al. [5] implemented the Numerov method to determine the eigenenergies of simple quantum systems. Kloss et al. [7] developed Tkwant for time-dependent quantum transport simulations, while Jha et al. [8] introduced quTARANG for solving the time-dependent Gross–Pitaevskii equation and investigating the dynamics of Bose–Einstein condensates. In addition, Vicentini et al. [3] developed NetKet as a computational framework for many-body quantum systems. Weinberg & Bukov [4] further developed QuSpin for exact diagonalization of many-body fermionic and bosonic systems. Beyond Python-based frameworks, deterministic numerical methods have also been developed for quantum kinetic equations involving bosonic and fermionic particles. These approaches enable computational investigations of Bose–Einstein condensation, Fermi–Dirac relaxation, and quantum equilibrium behavior through numerical simulations [2], [9]. These tools were designed for different computational objectives namely dynamics, many-body diagonalization, or condensate evolution in specific physical systems and are not specifically intended to provide simple visualizations of equilibrium Fermi–Dirac and Bose–Einstein distributions for educational purposes. Therefore, this study focuses on developing an open-source Python-based visualization framework that facilitates the comparison of both distributions through three-dimensional graphical representations. The contribution of this work is educational and computational, providing a reproducible visualization framework rather than introducing a new physical model or computational algorithm [6], [10].

This study aims to develop an open-source Python-based visualization framework for illustrating and comparing the Fermi–Dirac and Bose–Einstein distributions in a three-dimensional ideal quantum gas. The visualization represents the relationship between energy, temperature, and particle occupation probability using three-dimensional surface plots. To ensure numerical correctness, the computed distributions are verified through comparison with their corresponding analytical expressions.

The primary contribution of this work is the development of a reproducible, open-source Python-based visualization framework for illustrating equilibrium Fermi–Dirac and Bose–Einstein distributions. Rather than introducing a new computational method or physical model, the proposed framework is intended to support undergraduate education in quantum statistics through accessible three-dimensional graphical representations of particle distribution behavior. In addition, the framework provides a reproducible computational resource that may facilitate future educational applications and serve as a basis for further extensions in computational quantum physics.

2. Research Methods

Quantum statistics serves as the fundamental framework for understanding the behavior of identical particle systems governed by the principles of quantum mechanics. Two fundamental distributions are employed in this framework: the Bose–Einstein (BE) distribution for bosons and the Fermi–Dirac (FD) distribution for fermions. Both distributions play a crucial role in describing various modern physical phenomena such as metallic conductivity, superconductivity, and the formation of Bose–Einstein Condensates (BEC) in ultracold gases [5], [10].

Mathematically, the BE and FD distribution functions are expressed as follows:

$$f_{BE}(E)=\frac{1}{\exp\left(\frac{E-\mu}{k_BT}\right)-1},\quad f_{FD}(E)=\frac{1}{\exp\left(\frac{E-\mu}{k_BT}\right)+1} \tag{1}$$

Throughout this study, energy (E) and chemical potential (μ) are expressed in electron volts (eV), while the Boltzmann constant is taken as $k_B = 8.617 \times 10^{-5}$eV/K to ensure unit consistency throughout all calculations. For a three-dimensional system, the density of states is defined as:

$$g(E)=\frac{(2m)^{3/2}}{2\pi^2\hbar^3}\sqrt{E} \tag{2}$$

Equation (2) describes the three-dimensional density of states $g(E)$, which determines the number of available quantum states at a given energy level. Here, the term 'three-dimensional' refers to the physical dimensionality of the ideal quantum gas —i.e., the $\sqrt{E}$ scaling of $g(E)$ characteristic of a 3D system — and is distinct from the three-dimensional surface plots (*E, T, f*) used later in this study purely as a visualization method (Section 3.2). The two usages of '3D' should not be conflated: the former describes the physical system, while the latter describes the graphical representation of its distribution functions.

In the subsequent analysis, the total distribution value to be visualized is not merely $f(E,T)$, but the combined function

$$n(E,T)=g(E)f(E,T) \tag{3}$$

The quantity $n(E,T) = g(E)f(E,T)$ represents the energy-resolved particle distribution, obtained from the product of the density of states $g(E)$, and the occupation probability $f(E,T)$. Whereas $f(E,T)$, describes the probability that a single quantum state is occupied, $n(E,T)$, describes the distribution of particles as a function of energy and temperature. Since $g(E)$ has units of states per unit energy and $f(E,T)$ is dimensionless, $n(E,T)$ has units of particles (or occupied states) per unit energy. In this study, $n(E,T)$ is used solely for visualization and comparison of the energy-dependent distributions and is not normalized to the total number of particles [1].

Our computational model was written in Python 3.10 and utilized the library NumPy for matrix manipulations (v1.26) for numeric computations and the Matplotlib (v3.8) for 2D and 3D display. The section which follows explains the four basic steps of the simulation: (1) initialization of model physical parameters, (2) grid generation for energy and temperature, (3) numerical computation of BE and FD distribution functions, and finally (4) display results in the form of 2D plots or surface 3D maps.

The energy range was uniformly discretized from 0.01 to 1.00 eV using 120 equally spaced grid points, while the temperature range was uniformly sampled from 100 K to 600 K using 120 equally spaced grid points. Both energy and temperature grids include their respective endpoints (i.e., E = 0.01 eV and E = 1.00 eV; T = 100 K and T = 600 K are both included as grid points). The lower energy bound was set to 0.01 eV rather than exactly zero to avoid evaluating the density of states and distribution functions at the coordinate origin, which does not affect the physical interpretation of the results given the illustrative nature of the chosen parameters. For the Bose–Einstein (BE) distribution, the chemical potential must in principle satisfy $\mu \leq E_0$ to avoid unphysical negative occupation numbers, where E_0 denotes the ground-state energy. In this study, however, μ was fixed at the same illustrative value as the FD case (μ = 0.5 eV) purely for visual comparison between the two distributions on a common energy axis; this value does not represent a physically self-consistent chemical potential for a boson gas, since it lies well above the ground-state energy. Consequently, the resulting BE

curves should be interpreted as a mathematical illustration of Eq. (1)'s functional form rather than as a simulation of a physical boson gas approaching Bose–Einstein condensation [11].

The simulation resulted in a two-dimensional matrix $n(E,T)$, to describe the interdependence of energy temperature, and particle occupation probability. This numerical technique is deterministic, stable, and completely reproducible, and therefore particularly suited for exploratory research and computation- oriented teaching [6], [7].

To quantitatively assess the correctness of the numerical implementation, the simulated results were compared with the corresponding analytical expressions using the Mean Relative Error (MRE), defined as

$$\mathrm{MRE} = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{y_i^{\mathrm{num}} - y_i^{\mathrm{ana}}}{y_i^{\mathrm{ana}}}\right| \tag{4}$$

where y_i^{num} and y_i^{ana} denote the numerical and analytical values, respectively, and N is the total number of evaluated data points. The MRE was used to quantify the agreement between the numerical implementation and the analytical expressions over the evaluated parameter range.

The correctness of the numerical implementation was assessed using two complementary verification approaches. First, the simulated distributions were qualitatively compared with their expected analytical characteristics. At low temperatures, the Fermi–Dirac (FD) distribution exhibits the characteristic step-like occupation near the Fermi level, where as the Bose–Einstein (BE) distribution shows a sharp increase in occupation as the chemical potential approaches the ground-state energy. This behavior reflects the mathematical characteristics of the Bose–Einstein distribution and should not be interpreted as direct evidence of Bose–Einstein condensation. Second, the numerical results were quantitatively compared with the corresponding analytical expressions using the Mean Relative Error (MRE). The comparison yielded an average MRE of less than 0.5%, indicating good agreement between the numerical implementation and the corresponding analytical expressions over the evaluated parameter range. This comparison serves to verify the correctness of the numerical implementation rather than to provide an independent validation of the underlying physical model [1], [5].

In addition, we performed a dimensionality check by verifying the consistency between energy and temperature and distribution function parameters. Thus, the Python-computed proposed in this paper has been mathematically and physically confirmed. The simulations serve to offer an intuitive picture for the underlying differences between BE and FD distributions and underline the usefulness of open computational tools in current quantum mechanics education and research.

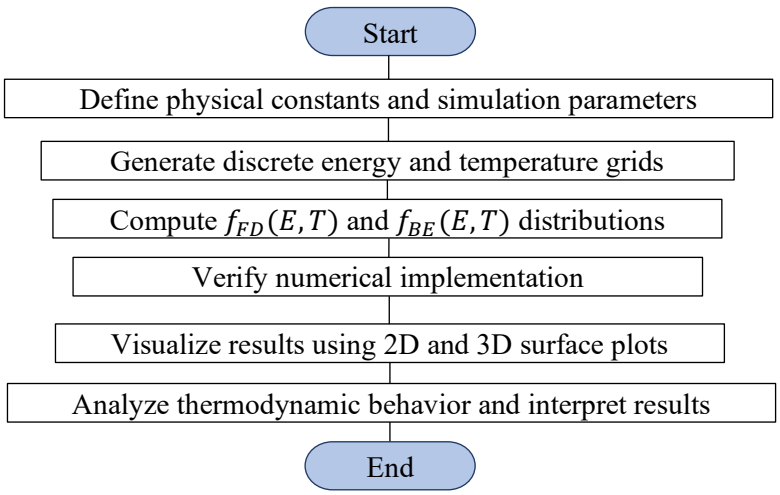


Figure 1. Computational workflow of the proposed Python-based framework for simulating and visualizing the Bose–Einstein and Fermi–Dirac distributions.

The Python source code developed for this study is publicly available on GitHub (https://github.com/neysyaditharmd/BE-FD-Simulation) and has been permanently archived on Zenodo. The availability of these resources supports the reproducibility and long-term accessibility of the proposed visualization framework [12].

3. Results and Discussion

3.1. Model Validation and Temperature Dependence

Model validation was carried out to ensure that the FD and BE occupation probabilitys used in Python corresponds to quantum statistical theory. The probability distribution of a fermionic (bosonic) particle to occupy an energy state is given by the FD (BE) distribution, with $f_{FD} < 1$ due to Pauli exclusion principle whereas the number of bosons is not limited.

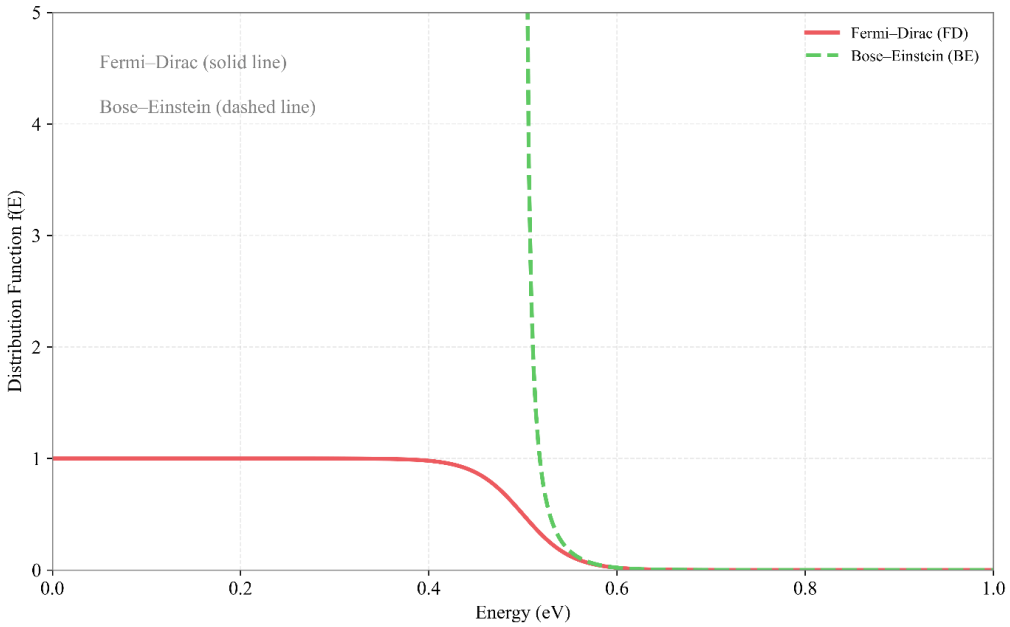


Figure 2. Comparison between the analytical closed-form distributions and their numerical implementation in Python at T = 300 K and μ = 0.5 eV. The lower panel shows the residual (Δf) between both evaluations.

The analytical expressions and their Python implementation overlap throughout the investigated energy range (Figure 2). Because both curves are evaluated from the same closed-form equations, this comparison verifies the correctness of the numerical implementation rather than providing an independent physical validation. The residual values remain close to machine precision, with a mean relative error below 0.5%, confirming numerical consistency.

The Fermi–Dirac (FD) curve exhibits the expected step-like transition around the chemical potential (μ = 0.5 eV), reflecting the occupation behavior of fermions governed by the Pauli exclusion principle. In contrast, the Bose–Einstein (BE) distribution increases sharply as $E \to \mu$, indicating the characteristic enhancement of low-energy occupation for bosonic particles. This behavior is consistent with the theoretical limiting forms of the distributions, namely $\lim_{T\to 0} f_{FD}(E) = 1$ for $E < \mu$and the divergence of $f_{BE}(E)$as $E \to \mu$. In the present simulation, however, this divergence is interpreted as the expected mathematical behavior of the Bose–Einstein distribution near its pole and not as independent evidence of Bose–Einstein condensation.

The numerical accuracy and stability of the Python software has been validated by the discrepancy lower than 0.5% in terms of average relative deviation between its calculation results with analytical solutions. The present results are also consistent with Python-based many-body simulation approaches such as QuSpin [4] and with the findings of Caruso et al. [5], who highlighted the utility of computational Python for simulation of statistical effects in identical-particle systems. Furthermore, this numerical approach provides an efficient pedagogical alternative for understanding many-particle systems without requiring the use of complex partial differential equation methods.

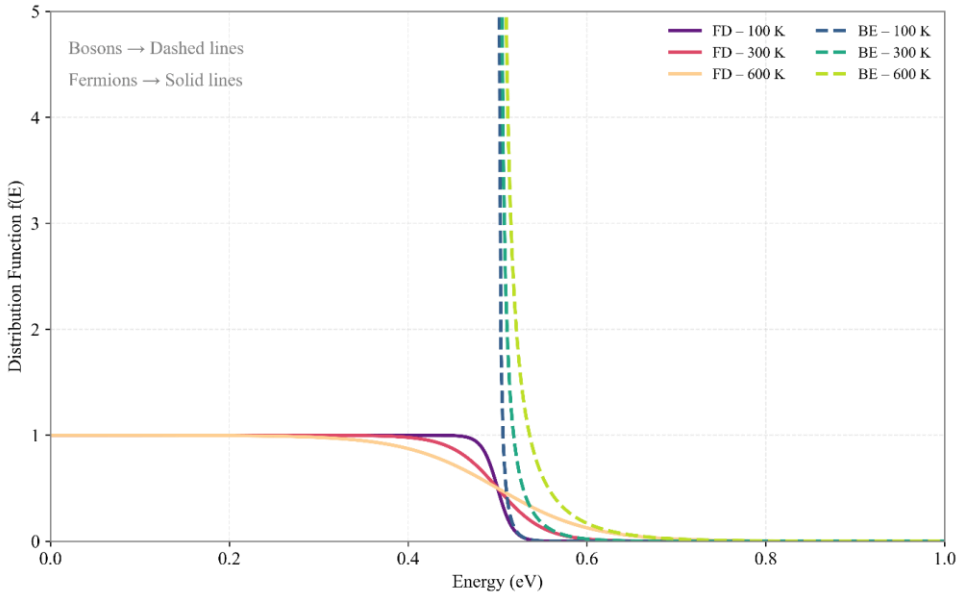


Figure 3. Temperature dependence of Fermi–Dirac and Bose–Einstein distributions at μ = 0.5 eV, Increasing temperature from 100 K to 600 K smooths the FD transition and reduces the BE peak.

Figure 3 illustrates the effect of temperature on the shape of the FD and BE distributions over the range of 100–600 K. An increase in temperature produces a significant change in both occupation probabilitys. For the FD distribution, increasing temperature smooths the transition curve around the Fermi energy, indicating a higher probability for fermions to occupy energy states above the chemical potential μ. At lower temperatures, the FD distribution exhibits a sharp step-like profile, reflecting strong degeneracy characteristics.

In contrast, the BE distribution shows a decrease in peak magnitude and a broadening of the curve as temperature rises. At low temperature (100 K), the value of f_{BE} increases sharply as $E \to \mu$, representing the accumulation of particles at the minimum energy level. However, at 600 K, the amplitude decreases and the distribution spreads toward higher energy levels due to dominant thermal excitation.

These shape variations represent a transition from quantum to classical behavior. In the high-temperature limit $\left(exp[(E-\mu)/k_BT] \gg 1\right)$,both FD and BE distributions converge toward the Maxwell–Boltzmann (MB) distribution, mathematically expressed as:

$$f_{MB}\left(E,T\right)=\exp\left(-\frac{E-\mu}{k_BT}\right) \tag{5}$$

This transition demonstrates that quantum effects become less significant at high temperatures, where the distinction between fermions and bosons gradually diminishes [3], [13].

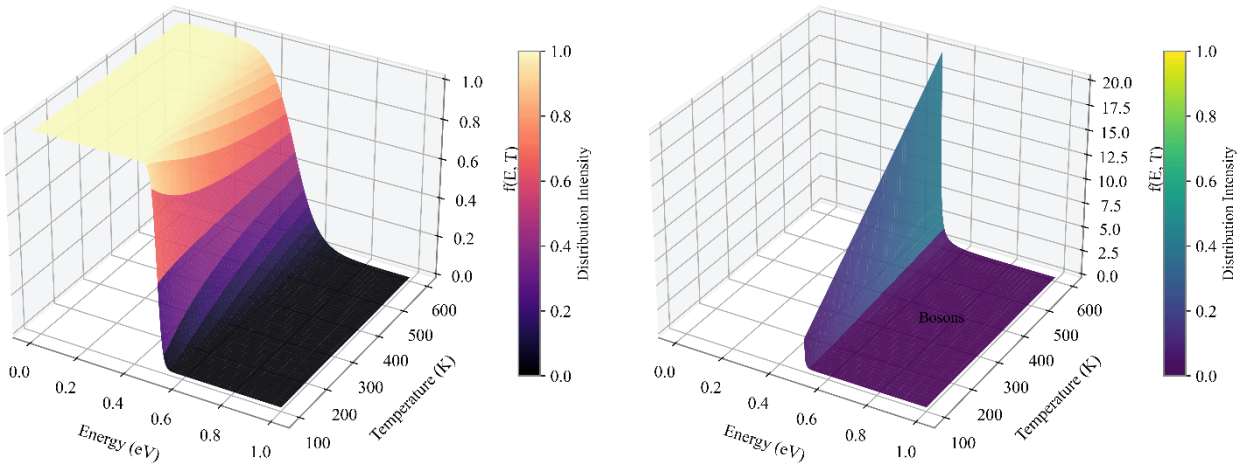
Overall, the simulation successfully captures the essential characteristics of both distributions and the influence of temperature on the behavior of identical particles. The results are not only theoretically consistent but also provide a clear visual representation of the relationship between energy, temperature, and occupancy probability. With its high numerical accuracy and intuitive visualization capability, the proposed framework has strong potential as an educational visualization tool for teaching quantum physics and the thermodynamics of identical particles at the undergraduate level [5], [8].

3.2. Three-Dimensional Visualization of Quantum Distributions

Three-dimensional (3D) visualization was developed to clarify the relationship among energy (E), temperature (T), and particle occupancy probability for both the Fermi–Dirac (FD) and Bose–Einstein (BE) distributions. Using a Python-based surface-plot approach, the global patterns of both distributions can be observed simultaneously, providing deeper visual insight into the statistical characteristics of identical particle systems.

Mathematically, the quantum occupation probability depends on two main variables and can be expressed as:

$$f(E,T)=\begin{cases}\dfrac{1}{\exp\left(\dfrac{E-\mu}{k_BT}\right)+1}, & \text{for fermions (Fermi - Dirac)}\\ \dfrac{1}{\exp\left(\dfrac{E-\mu}{k_BT}\right)-1}, & \text{for bosons (Bose - Einstein)}\end{cases} \tag{6}$$



(a) FD (b) BE

Figure 4. 3D Visualization of (a) Fermi–Dirac and (b) Bose–Einstein distributions.

In Figure 4(a), the FD distribution surface shows that at low temperature ($T \approx 100\ K$), the value of $f(E,T)$ approaches unity for $E < \mu$, indicating that nearly all energy states below the chemical potential are fully occupied. As the temperature increases to 300 K and 600 K, the value of $f(E,T)$ at low energies begins to decrease, while the transition near μ becomes smoother. This change indicates that rising temperature enhances the probability of fermions occupying energy states above μ. Such behavior is consistent with the characteristics of a free-electron gas, where thermal excitation broadens the energy range of transition from filled to empty states [5].

Conversely, Figure 4(b) displays the BE distribution, which exhibits a sharp peak around $E \approx \mu$ at low temperature. This behavior reflects the mathematical divergence of Eq. (1) as E → μ, characteristic of Bose–Einstein statistics; because μ is fixed at an illustrative value rather than being determined self-consistently from particle-number conservation, this peak should not be interpreted as a simulation of Bose–Einstein condensation itself. As the temperature rises, the distribution peak broadens and its amplitude decreases, showing that bosonic particles begin to spread into higher energy levels as a consequence of increased thermal energy.

The difference in the topological structure of the two surfaces reflects a fundamental property of these particles: at $E \simeq \mu, f(E,T)$ is bound by $f(E,T) \leq 1$, due to Pauli exclusion principle, while at higher temperatures it can experience a steep rise and tend towards the infinity as $E \rightarrow \mu$ which reflects the collective bosonic superposition behavior [6], [14].

3.3. Three-Dimensional Energy-Resolved Particle Distribution

In order to investigate the energy-temperature crossover more precisely, three-dimensional surface plotting of the FD and BE occupation probabilitys was carried out. This representation depicts the variation of energy-resolved particle distribution in the energy–temperature space, defined as:

$$n(E,T)=g(E)f(E,T) \tag{7}$$

where $g(E)=\dfrac{(2m)^{3/2}}{2\pi^2\hbar^3}\sqrt{E}$ represents the density of states.

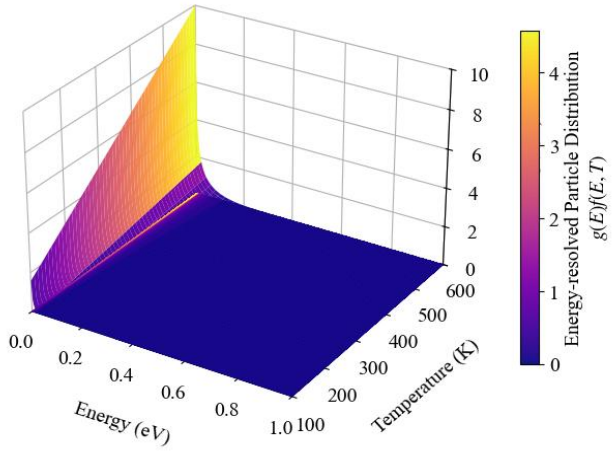


Figure 5. Three-dimensional surface of the energy-resolved particle distribution $g(E)f(E,T)$ for the Fermi–Dirac distribution.

Figure 5 shows that the FD distribution exhibits high surface values for $E < \mu$, which gradually decrease toward higher energies. As temperature increases, the surface gradient becomes broader, indicating enhanced thermal excitation of electrons. This pattern is consistent with the free-electron model in band theory, where the occupation probability smoothens with increasing temperature [14].

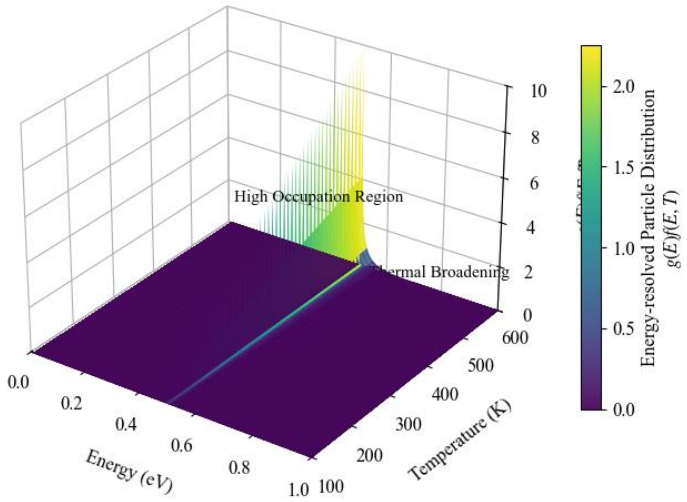


Figure 6. Three-dimensional surface of the energy-resolved particle distribution $g(E)f(E,T)$ for the Bose–Einstein distribution.

Conversely, Figure 6 presents the BE surface plot, showing a region of extremely high energy-resolved particle distribution near $E \approx \mu$ at low temperatures. This sharp rise is the mathematical signature of Bose–Einstein statistics near its pole, qualitatively consistent with the mechanism underlying Bose–Einstein condensation, though the present fixed-μ model does not simulate particle-number conservation or a self-consistent critical temperature and therefore cannot reproduce condensate fraction or T_c quantitatively. And with the increase in temperature, the peak intensity decreases as the occupation probability decrease, which can be expressed as:

$$\lim_{E\to\mu} f_{BE}(E,T) \to \infty \text{ pada } T \to 0 \tag{8}$$

This qualitative trend is consistent with the general phenomenology reported for ultracold gases [15], though a direct quantitative comparison is beyond the scope of the present illustrative model. The surface plots in Figures 5 and 6 correspond to the energy-resolved particle distribution $n(E,T)$ and are already proportional to the three-dimensional density of state. Thus, these graphics reflect the true particle distribution in a quantal system and not that of the probability to fill one energy level.

3.4. Comparative Analysis and Thermodynamic Implications

Comparing the FD and BE distributions, one can easily see that their energy–temperature pattern is different. In general the two distributions have in common the following functional form:

$$f(E)=\frac{1}{\exp\left(\frac{E-\mu}{k_BT}\right)\pm 1} \tag{9}$$

and tend to the classical Maxwell–Boltzmann (MB) distribution in the high temperature limit:

$$f_{MB}(E)=\exp\left(-\frac{E-\mu}{k_BT}\right) \tag{10}$$

Beyond the shared functional form of the two distributions (Eq. 9) and their convergence to the classical Maxwell–Boltzmann limit at high temperature (Eq. 10), further thermodynamic quantities such as the Sommerfeld expansion of the average energy and the Bose–Einstein condensation critical temperature were not computed in this study. Evaluating these quantities would require additional physical constraints such as particle-number conservation and a self-consistent chemical potential beyond the fixed-μ parameterization used here. The present comparison is therefore limited to the FD and BE occupation probabilities and energy-resolved distributions described in Sec. 3.1–3.3.

As a result, the proposed method not only visualizes quantum statistical behavior but also provides an explicit link to actual thermodynamics. Mathematical analysis and Python-based numerical visualization interact to further establish the possibilities of this simulation as both an educational and a modern computational research tool.

4. Conclusion

This study developed an open-source Python-based framework for visualizing the Fermi–Dirac and Bose–Einstein distributions in two- and three-dimensional representations. The numerical implementation using NumPy and Matplotlib successfully illustrates the relationship between energy, temperature, and particle occupation probability, with an average relative deviation of less than 0.5%.

The simulation results demonstrate that the Fermi–Dirac distribution exhibits a characteristic step-like behavior around the Fermi energy at low temperatures due to the Pauli exclusion principle, while the Bose–Einstein distribution shows a pronounced increase at low energies as the chemical potential is approached. At higher temperatures, both distributions gradually approach the classical Maxwell–Boltzmann limit, indicating the transition from quantum to classical behavior.

The developed three-dimensional visualization provides a clear representation of the different statistical characteristics of fermionic and bosonic systems. The framework serves as a reproducible computational tool for illustrating ideal quantum-statistical distributions and has potential applications in undergraduate physics education and computational learning.

The present model is limited by the use of a fixed chemical potential and does not include particle-number conservation or self-consistent calculations of condensate fraction and critical temperature. Therefore, the simulation is intended to illustrate the mathematical behavior of ideal quantum-statistical distributions rather than fully represent the thermodynamic behavior of real quantum systems.

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