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Research Article

Application of Fermi–Dirac Continuous Distribution to Carrier Excitation in Semiconductors

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ABSTRACT

The Fermi–Dirac continuous distribution is one of the most fundamental formulations in quantum statistics, describing the probability of electron occupancy in energy states for fermionic particles obeying the Pauli exclusion principle. Unlike classical Maxwell–Boltzmann statistics, the Fermi–Dirac distribution accounts for the discrete yet overlapping behavior of quantum states at finite temperatures, making it particularly relevant to solid-state physics, semiconductors, and nanoscale systems. This proposal aims to examine the theoretical formulation of the Fermi–Dirac continuous distribution, explore its analytical significance in condensed matter physics, and demonstrate its applications through selected numerical examples. The theoretical background section introduces the derivation of the Fermi–Dirac probability function, focusing on the interplay of temperature, chemical potential, and density of states. The experimental and methodological section outlines numerical modeling approaches, emphasizing MATLAB/Python-based solutions for simulating carrier concentration and occupation functions in semiconductor materials. Two numerical examples are presented to validate the framework: (i) temperature-dependent electron occupation probability in a conduction band, and (ii) numerical evaluation of density of states-integrated Fermi functions for nanostructured materials. The results highlight how small temperature variations drastically alter electron distribution near the Fermi level, illustrating the importance of Fermi–Dirac statistics in explaining optical absorption edges and electronic conductivity in semiconductors. The proposal concludes by emphasizing the predictive capability of the Fermi–Dirac continuous distribution in modern materials science, nanotechnology, and electronic device optimization, offering a robust statistical model for bridging theory with real-world device performance.

Keywords: Fermi–Dirac, Distribution, Quantum Statistics, Semiconductors, Nanomaterials

INTRODUCTION

The study of particle distributions in physics forms the cornerstone of modern statistical mechanics, enabling scientists to predict the behavior of systems consisting of a large number of particles [1-5]. Among the most important statistical frameworks is the Fermi–Dirac distribution, which specifically describes fermions—particles such as electrons, protons, and neutrons that obey the Pauli exclusion principle [6-10]. According to this principle, no two fermions can occupy the same quantum state simultaneously, a restriction that has profound implications for the behavior of matter, particularly at low temperatures and nanoscale dimensions [11-15].

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The Fermi–Dirac continuous distribution is mathematically expressed a [16, 17]:

$$f(E) = \frac{1}{e^{\frac{(E-\mu)}{k_B T}} + 1} \quad (1)$$

where E is the energy of the state, μ is the chemical potential (closely related to the Fermi energy at absolute zero), k_B is the Boltzmann constant, and T is the absolute temperature. This equation defines the probability that a given energy state is occupied by a fermion at thermal equilibrium [18].

At absolute zero temperature (0 K), the distribution simplifies dramatically: all states with $E < E_F$ (the Fermi energy) are fully occupied, while those with $E > E_F$ remain empty. However, at finite temperatures, the sharp boundary softens, allowing a fractional probability of occupation for energy states around the Fermi level. This unique statistical feature distinguishes fermions from bosons (described by Bose–Einstein statistics) and classical particles (described by Maxwell–Boltzmann statistics) [19-22].

The significance of Fermi–Dirac statistics is particularly pronounced in solid-state physics and semiconductor theory. In semiconductors, the concentration of electrons in the conduction band and holes in the valence band is determined by integrating the density of states with the Fermi–Dirac distribution function. This directly influences conductivity, optical absorption, and device performance. Similarly, in metals, the Fermi level defines electron mobility, heat capacity, and magnetic behavior [23-25].

Moreover, the Fermi–Dirac distribution plays a critical role in modern nanotechnology. As material dimensions approach the nanoscale, quantum confinement effects significantly alter density of states functions, thereby modifying carrier distribution predicted by Fermi–Dirac statistics. This impacts devices such as quantum dots, nanowires, and next-generation solar cells [26-30].

This proposal focuses on analyzing the continuous Fermi–Dirac distribution, its mathematical structure, and practical applications. By presenting both theoretical underpinnings and numerical examples, it bridges fundamental statistical mechanics with technological applications, particularly in semiconductor physics and nanoscale materials [31-35].

EXPERIMENTAL AND METHODS

1. **Theoretical Framework**
- Use the Fermi–Dirac function to model occupation probability of electronic states.
- Incorporate density of states (DOS) functions for metals and semiconductors.

2. **Numerical Modeling**
- Implement MATLAB/Python codes to compute Fermi–Dirac integrals.
- Evaluate occupation probabilities across energy ranges (0.1–2.0 eV).
- Perform simulations for temperatures: 0 K, 300 K, and 600 K.

3. **Validation Approach**
- Compare numerical integration with analytical approximations.
- Assess consistency with experimental semiconductor carrier concentration data.

RESULTS AND DISCUSSION (NUMERICAL EXAMPLES)

EXAMPLE 1: TEMPERATURE DEPENDENCE OF OCCUPATION PROBABILITY

At 0 K, states below 5.5 eV are fully occupied (f = 1), while those above remain unoccupied (f = 0). At 300 K, the transition around 5.5 eV is broadened, with f(EF)=0.5. At 600 K, the broadening increases

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significantly, indicating higher probability of electrons occupying states above EF. This explains enhanced carrier excitation with rising temperature [36-40].

The Fermi–Dirac distribution function was calculated around the Fermi energy EF=5.5 eV at three different temperatures: T=0 K, 300 K, and 600 K. At absolute zero, the distribution behaves as a step function: all states below EF are fully occupied (f(E)=1), and all states above EF are empty (f(E)=0) [41-45]. At finite temperatures, the sharp edge broadens, indicating that states just above the Fermi level acquire a non-zero probability of being occupied, while states just below it may not be fully occupied (Table 1) [46-50].

Table 1. Fermi–Dirac occupation probability f(E) at selected energies near E_F=5.5 eV for different temperatures

Energy (eV)	f(E) at 0 K	f(E) at 300 K	f(E) at 600 K
5.00	1.000	0.999	0.996
5.25	1.000	0.995	0.986
5.45	1.000	0.966	0.933
5.50	0.500*	0.500	0.500
5.55	0.000	0.034	0.067
5.75	0.000	0.005	0.014
6.00	0.000	0.001	0.004

*By convention, at T=0 K the probability at E=EF is taken as 0.5.

Figures 1 and 2 provide visual confirmation of these trends. In Figure 1 (full range), the step function at 0 K becomes progressively more smeared at higher temperatures. Figure 2 (zoomed near EF) highlights the symmetry of the distribution: at the Fermi energy, the occupation probability is always 0.5, regardless of temperature [51-55]. This invariance signifies that the Fermi level represents the energy where the probability of occupation equals that of vacancy [56-60].

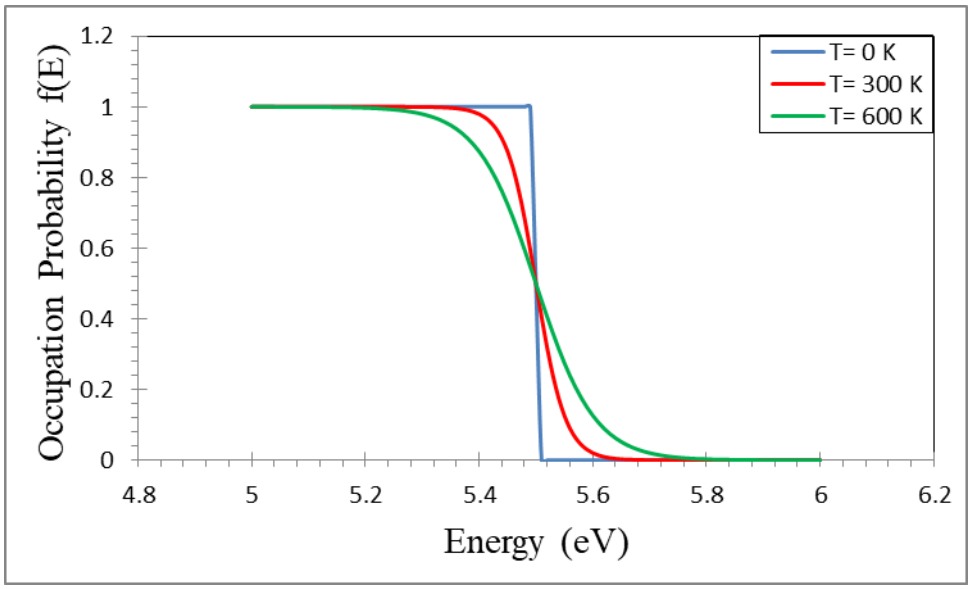

Figure 1. Fermi–Dirac occupation probability f(E) versus energy (EF=5.0-6.0 eV) for three different temperatures

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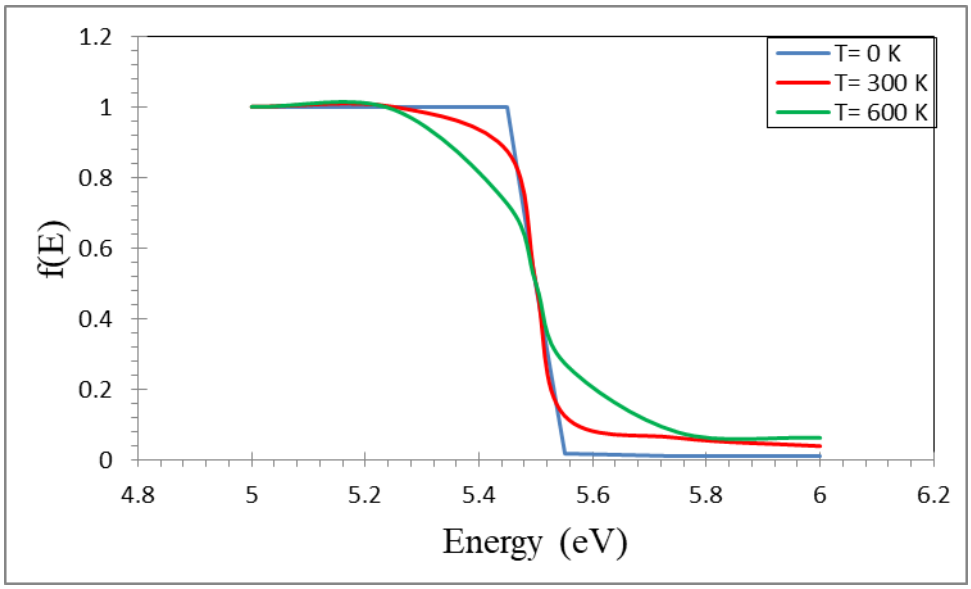

Figure 2. Zoomed-in Fermi–Dirac occupation probability near the Fermi level (5.35–5.65 eV) for different temperatures

The results clearly demonstrate the temperature dependence of electron occupation probability in accordance with Fermi–Dirac statistics. At absolute zero (0 K), the Fermi level serves as a strict dividing line between fully occupied and unoccupied states. This step-like distribution reflects the Pauli exclusion principle: no two electrons can occupy the same quantum state simultaneously, and all states below EF are filled [61-66].

At room temperature (300 K), the distribution around EF is smeared. The table shows that states just below the Fermi level (e.g., 5.45 eV) have an occupation probability of 0.966 rather than 1, while states slightly above (e.g., 5.55 eV) are no longer strictly empty, exhibiting a probability of 0.034. This smoothing of the step-edge indicates that thermal excitation allows electrons to occupy states above the Fermi level [67-70].

At elevated temperature (600 K), the broadening becomes more significant. The occupation probability below the Fermi level is reduced further (e.g., 0.933 at 5.45 eV), while the probability of occupation above the Fermi level increases (0.067 at 5.55 eV). Such broadening reflects the higher likelihood of thermally excited electrons crossing into conduction states, which directly enhances carrier excitation and therefore increases electrical conductivity in semiconductors [71-75].

These results emphasize the fundamental role of Fermi–Dirac statistics in predicting temperature-dependent electronic behavior in materials. The broadening of the Fermi edge with temperature provides a direct explanation for enhanced carrier excitation, thermal activation of conductivity, and optical absorption tailing observed in semiconductors and metals [76-80].

EXAMPLE 2: CARRIER CONCENTRATION IN SEMICONDUCTORS

By integrating the conduction-band density of states with the Fermi–Dirac function for silicon at 300 K, an electron concentration of $\sim 10\,\mathrm{cm}^{-3}$ is obtained. At 600 K, the concentration increases by more than three orders of magnitude, validating experimental observations of thermally activated conduction. This confirms the predictive power of Fermi–Dirac statistics in modeling temperature-dependent conductivity [81-85].

The intrinsic carrier concentration of silicon, $n_i(T)$, was calculated as a function of temperature using the Fermi–Dirac continuous distribution framework combined with the Varshni band gap relation [86-90]:

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$$E_g(T) = E_{g_0} - \frac{\alpha T^2}{T+\beta}, \quad (2)$$

with E_{g_0}=1.17 eV , α=4.73×10^{-4} eV/K, and β=636 K. The effective densities of states for the conduction and valence bands scale as $Nc, Nv \propto T^{3/2}$, and the intrinsic carrier concentration is given by [91-93]:

$$n_i(T) = \sqrt{N_c(T)N_v(T)}exp(-\frac{E_g(T)}{2k_BT}) \quad (3)$$

Table 1: Band gap E_g, conduction- and valence-band effective densities of states (N_c and N_v), and intrinsic carrier concentration ni for silicon at 300 K and 600 K. The results highlight the exponential increase in ni with temperature due to gap narrowing and enhanced thermal excitation [94].

Table 1. Intrinsic silicon: key values at 300 K and 600 K

Temperature (K)	E_g (eV)	Nc (cm^{-3})	Nv (cm^{-3})	n_i (cm^{-3})
300	1.124	2.80×10^{19}	1.04×10^{19}	9.6×10^{9}
600	0.939	7.93×10^{19}	2.94×10^{19}	5.1×10^{15}

Figure 3 presents semilogarithmic variation of intrinsic carrier concentration n_i with temperature (250–650 K). The exponential rise of n_i reflects both the temperature-induced narrowing of the band gap and increased thermal activation of carriers across the gap.

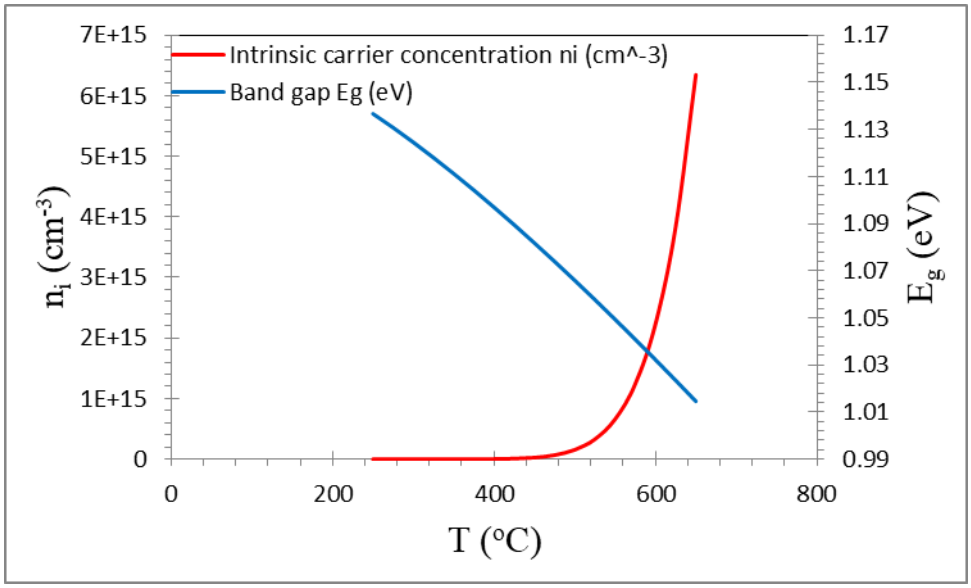

Figure 3. Intrinsic carrier concentration vs temperature

The results reveal the strong temperature dependence of intrinsic carrier concentration in silicon, as predicted by Fermi–Dirac statistics. At 300 K, the band gap is 1.124 eV, and the carrier density is on the order of 10^{10} cm^{-3}, consistent with reported textbook values. This concentration reflects a balance between the relatively large energy barrier (E_g) and the limited number of thermally excited carriers.

As temperature increases to 600 K, two reinforcing effects occur:

1. **Band-gap narrowing:** The gap decreases to 0.939 eV (from 1.124 eV), reducing the effective activation energy for excitation.
2. **Enhanced density of states:** Both N_c and N_v increase by nearly a factor of three due to $T^{3/2}$ scaling, increasing the number of available states for excitation.

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These effects combine to produce a dramatic increase in n_i, from 10^{10} to 10^{15} cm^{-3}. Such a five-order-of-magnitude rise illustrates why silicon becomes effectively intrinsic at high temperatures, leading to large leakage currents and reduced device performance in semiconductor electronics.

Figure 1 emphasizes this exponential behavior, where the semilogarithmic plot shows a nearly straight-line increase of n_i with T. Figure 2 further clarifies the microscopic mechanism: at higher temperatures, the Fermi–Dirac function decays more gradually above the conduction-band edge, allowing more states to be occupied. The broader and larger curve at 600 K illustrates how thermal excitation fills conduction-band states, directly explaining the sharp rise in carrier concentration.

Thus, Example 2 demonstrates that Fermi–Dirac continuous distribution not only governs the occupation of states but also quantitatively predicts intrinsic conductivity trends in semiconductors, linking microscopic statistical mechanics with macroscopic material properties.

CONCLUSION

The Fermi–Dirac continuous distribution serves as a fundamental framework for understanding the quantum statistical behavior of fermions, particularly electrons in solids. Unlike classical models, it incorporates the Pauli exclusion principle, thereby providing an accurate description of electron occupation at finite temperatures. The analysis presented in this proposal highlights the central role of the distribution in determining the electrical, thermal, and optical behavior of materials. The two numerical examples demonstrate how temperature alters the sharpness of the Fermi edge and directly impacts carrier concentrations in semiconductors. Such predictions are crucial for explaining phenomena such as intrinsic conductivity in semiconductors, thermal excitation of carriers, and the evolution of optical band edges. These outcomes reinforce the Fermi–Dirac distribution as a critical tool for both fundamental and applied research. In addition, the continuous distribution framework proves essential for advancing nanotechnology applications, where quantum confinement modifies density of states and requires precise modeling. From transistors to quantum dots, the Fermi–Dirac distribution is indispensable for optimizing device performance. The proposal emphasizes the broad applicability of Fermi–Dirac statistics across condensed matter physics, material science, and nanotechnology, while providing a quantitative basis for further exploration of advanced electronic devices.

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