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On the Analytical Determination of the Seebeck Coefficient Using the Fermi–Dirac Approximation

The Seebeck coefficient, or thermoelectric power, is a key physical parameter that quantifies the voltage generated in response to a temperature gradient across a material. Accurate evaluation of this coefficient is essential in order to optimize the performance of thermoelectric devices. This study proposes a theoretical approach to the analytical determination of the Seebeck coefficient in semiconductors, based on the Fermi–Dirac statistical approximation. The model incorporates the temperature dependence of the Fermi level, which introduces an intrinsic gradient along the thermoelectric structure under non-equilibrium thermal conditions. This framework enables a more precise understanding of the interplay between the carrier distribution, energy levels, and temperature variation. The analytical expressions obtained here show good agreement with the results of numerical methods, and offer significant advantages in terms of modeling and designing high-performance thermoelectric materials. The proposed approach proves to be an efficient and insightful tool for theoretical investigations and optimization studies in semiconductor thermoelectrics.

Keywords: Seebeck coefficient; thermoelectric power; semiconductor; Fermi–Dirac method

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Introduction

Thermoelectric effects, which are primarily quantified by the Seebeck coefficient, involve direct interconversion between thermal and electrical energy in a material system. The Seebeck effect refers to a phenomenon where a temperature gradient established along a thermoelectric material induces an electric potential difference, and vice versa, and this forms the foundational principle behind thermoelectric generators and coolers [1–7]. The efficiency of these energy conversion processes is strongly governed by the magnitude and behavior of the Seebeck coefficient indifferent materials and temperature regimes.

In semiconductors and complex materials, the Seebeck coefficient is particularly sensitive to microscopic interactions involving charge carriers. These include carrier–carrier, carrier–phonon, and in the case of magnetic semiconductors, carrier–localized magnetic moment interactions. Such interactions can significantly alter the distribution function of carriers, leading to notable changes in the thermoelectric response. For example, scattering mechanisms impose constraints on the final states that carriers can occupy, often resulting in a reduction of the Seebeck coefficient due to the suppression of entropy transport per carrier [8, 9].

The Seebeck coefficient is not solely a material constant, and is closely associated with the carrier concentration, effective mass, and temperature, all of which affect the position and dynamics of the Fermi level. In degenerate or heavily doped semiconductors in particular, where classical (Boltzmann) statistics become insufficient, a quantum-statistical approach becomes necessary. The Fermi–Dirac distribution provides a more accurate description of carrier occupancy in such systems, and is essential in order to capture realistic transport behavior [10, 11]. The Gaussian density of states (DOS) approximation is also widely used to model disordered or amorphous semiconductors and organic materials, in which the electronic states are not sharply defined due to substantial energetic disorder. Unlike crystalline semiconductors, which have well-defined band structures derived from periodic Bloch states, disordered systems lack long-range structural order. This absence of periodicity results in localized electronic states with broadened energy levels, due to variations in the local environment such as structural distortions or fluctuations in molecular orientation [12–14].

In this study, we present an analytical approach for evaluating the Seebeck coefficient in semiconducting materials within the framework of a Gaussian DOS and the Fermi–Dirac statistical approximation. The use of the Gaussian approximation for the DOS is physically justified in systems where energetic disorder dominates, such as amorphous and organic semiconductors. In these materials, the absence of long-range order leads to a broadening of the electronic energy levels, which can be effectively modeled by a Gaussian distribution. This approximation is commonly accepted for disordered systems, including amorphous silicon, disordered metal oxides, and organic semiconductors, where localized states and site-to-site energy fluctuations govern the charge transport [15–18]. To incorporate the temperature dependence of the chemical potential (Fermi level), we used a numerical method in Mathematica 10.0 that is valid across both non-degenerate and degenerate regimes. This theoretical framework enables improved insight into the thermoelectric properties of materials without relying solely on numerical simulations. The analytical results obtained here demonstrate the reliability and applicability of the proposed method for thermoelectric modeling.

Proposed Method and Formulae

An analytical formula was proposed in [19–23] for the calculation of the Seebeck coefficient, as presented below:

$$S = -\frac{eL^2}{\tau T\sigma}\int_{-\infty}^{\infty}\frac{E-E_f}{kT}f(E,T)(1-f(E,T))N(E)dE\,, \tag{1}$$

where σ is the electrical conductivity, τ is the scattering time, $L^2 = \frac{1}{3}(\tau\vartheta)^2$ is the scattering distance (mean free path), *N(E)* is the DOS, which can be represented by a Gaussian function, and *f*(*E*) is the Fermi–Dirac distribution function. These quantities are defined as follows [20]:

$$N(E) = \frac{N_0}{\sqrt{2\pi}\delta}e^{-\frac{1}{2}\left(\frac{E-E_0}{\delta}\right)^2} \tag{2}$$

and

$$f(E) = \frac{1}{1+e^{\frac{E-E_f}{kT}}}\,, \tag{3}$$

where the energy E_0 is defined as the center of the Gaussian distribution, N_0 is the total concentration of energetic states, and δ is the width of the distribution. Substituting Eqs. (2) and (3) into Eq. (1) gives the following expression:

$$S = -\frac{eL^2}{\sigma\tau kT^2}\frac{N_0}{\sqrt{2\pi}\delta}\int_{-\infty}^{\infty}\frac{1}{1+e^{\frac{E-E_f}{kT}}}\left(1-\frac{1}{1+e^{\frac{E-E_f}{kT}}}\right)(E-E_f)e^{-\frac{1}{2}\left(\frac{E-E_0}{\delta}\right)^2}dE\,, \tag{4}$$

where σ is the conductivity of the material. Eq. (4) can be expressed in the following form:

$$S = -\frac{eL^2}{\sigma\tau kT^2}\frac{N_0}{\sqrt{2\pi}\delta}Q(k,\delta,T,E_f,E_0)\,, \tag{5}$$

where

$$Q(k,\delta,T,E_f,E_0) = \int_{-\infty}^{\infty}\frac{1}{1+e^{\frac{E-E_f}{kT}}}\left(1-\frac{1}{1+e^{\frac{E-E_f}{kT}}}\right)(E-E_f)e^{-\frac{1}{2}\left(\frac{E-E_0}{|\delta|}\right)^2}dE\,. \tag{6}$$

Due to the complexity of Eq. (6), the derivation of a closed-form analytical expression is highly challenging; it is therefore expressed as a sum of simpler integrals, in the following form:

$$Q(k,\delta,T,E_f,E_0) = L(k,\delta,T,E_f,E_0) + M(k,\delta,T,E_f,E_0) - R(k,\delta,T,E_f,E_0) - K(k,\delta,T,E_f,E_0)\,, \tag{7}$$

where

$$L(k,\delta,T,E_f,E_0) = \int_{0}^{E_f}\frac{(E-E_f)}{1+e^{\frac{E-E_f}{kT}}}e^{-\frac{1}{2}\left(\frac{E-E_0}{\delta}\right)^2}dE\,, \tag{8}$$

$$M(k,\delta,T,E_f,E_0)=\int_{E_f}^{\infty}\frac{(E-E_f)}{1+e^{\frac{E-E_f}{kT}}}e^{-\frac{1}{2}\left(\frac{E-E_0}{\delta}\right)^2}dE\,, \tag{9}$$

$$R(k,\delta,T,E_f,E_0)=\int_{0}^{\infty}\frac{(E+E_f)}{1+e^{-\frac{E+E_f}{kT}}}e^{-\frac{1}{2}\left(\frac{E+E_0}{|\delta|}\right)^2}dE\,, \tag{10}$$

$$K(k,\delta,T,E_f,E_0)=\int_{-\infty}^{\infty}\frac{(E-E_f)}{\left(1+e^{\frac{E-E_f}{kT}}\right)^2}e^{-\frac{1}{2}\left(\frac{E-E_0}{|\delta|}\right)^2}dE\,. \tag{11}$$

As an be seen from Eq. (5), the determination of the Seebeck coefficient depends on the accurate evaluation of Eqs. (8)–(11). To derive ananalytical expression from Eqs. (8)–(11), the binomial expansion theorem and the exponential series expansion are employed, as follows [24, 25]:

$$e^{\pm x}=\sum_{i=0}^{\infty}(\pm 1)^i\,\frac{x^i}{i!} \tag{12}$$

and

$$(x\pm y)^n=\begin{cases}\lim\limits_{N\to\infty}\sum_{m=0}^{N}(\pm 1)^m f_m(n)x^{n-m}y^m \text{ for noninteger } n \text{ and } x\ge y\\ \sum_{m=0}^{n}(\pm 1)^m f_m(n)x^{n-m}y^m \text{ for integer } n\end{cases} \tag{13}$$

where $f_m(n)$ are binomial coefficients defined by:

$$f_m(n)=\frac{1}{m!}\prod_{i=0}^{m-1}(n-i)\,. \tag{14}$$

By substituting Eqs. (12) and (13) into Eqs. (8)–(10), a general analytical expression for $L(k,\delta,T,E_f,E_0)$, $M(k,\delta,T,E_f,E_0)$ and $R(k,\delta,T,E_f,E_0)$ can be derived as follows:

$$L(k,\delta,T,E_f,E_0)=\lim_{N\to\infty}\sum_{i=0}^{N}\frac{(-1)^i}{(2\delta^2)^i\,i!}\sum_{j=0}^{2i}(-1)^j f_j(2i)E_0^j H_{2i-j}(k,T,E_f)\,; \tag{15}$$

$$M(k,\delta,T,E_f,E_0)=\lim_{N'\to\infty}\sum_{i=0}^{N'}f_i(-1)\,\mathrm{Exp}\left(\frac{E_f(i+1)}{kT}-\frac{E_0^2}{2\delta^2}\right)T\left(E_f,\frac{1}{2\delta^2},-\frac{E_0^2}{\delta^2}+\frac{i+1}{kT}\right) \tag{16}$$

$$R(k,\delta,T,E_f,E_0)=\lim_{N\to\infty}\sum_{i=0}^{N'}f_i(-1)\,\mathrm{Exp}\left(-\frac{E_f i}{kT}-\frac{E_0^2}{2\delta^2}\right)S_i\left(E_f,\frac{1}{2\delta^2},\frac{E_0}{\delta^2}\right) \tag{17}$$

$$H_n(k,T,E_f)=\int_{0}^{E_f}\frac{(E-E_f)E^n}{1+e^{\frac{E-E_f}{kT}}}dE \tag{18}$$

$$T(p,q,b)=\frac{e^{-p(b+pq)}}{4\sqrt{q^3}}\left(2\sqrt{q}-e^{\frac{(b+2pq)^2}{4q}}\sqrt{\pi}(b+2pq)Erfc\left(\frac{b+2pq}{2\sqrt{q}}\right)\right) \tag{19}$$

$$S_i\left(p,q,b\right)=\begin{cases}\dfrac{2\sqrt{q}-\sqrt{\pi}e^{\frac{b^2}{4q}}(b-2pq)Erfc\left(\dfrac{b}{2\sqrt{q}}\right)}{4\sqrt{q^3}} & \text{for}\quad i=0\\ \dfrac{1}{4}\lim\limits_{N\to\infty}\sum\limits_{j=1}^{N}\dfrac{(-1)^j}{j!}\left(\dfrac{i}{kT}\right)^j q^{-\frac{1}{2}(3+j)}\left(2\sqrt{q}\Gamma(j/2+1)\left({}_1F_1\left(\dfrac{2+j}{2},\dfrac{1}{2},\dfrac{b^2}{4q}\right)-\right.\right. & \\ \left.-bp\,{}_1F_1\left(\dfrac{2+j}{2},\dfrac{3}{2},\dfrac{b^2}{4q}\right)\right)+\Gamma\left(\dfrac{j+1}{2}\right)\left(2pq\,{}_1F_1\left(\dfrac{1+j}{2},\dfrac{1}{2},\dfrac{b^2}{4q}\right)-b(j+1)\times\right. & \\ \left.\left.\times{}_1F_1\left(\dfrac{3+j}{2},\dfrac{3}{2},\dfrac{b^2}{4q}\right)\right)\right) & \text{for}\quad i\neq 0\end{cases}\tag{20}$$

where the parameters N and N' are the upper limits of the summations. The quantities $\Gamma(x)$ and $Erfc(x)$ are defined as follows:

$$\Gamma(x)=\int_0^{\infty}t^{\alpha-1}e^{-t}dt\,,\tag{21}$$

$$Erfc(x)=\frac{2}{\sqrt{\pi}}\int_x^{\infty}e^{-t^2}dt\,.\tag{22}$$

Note that the functions $K(k,\delta,T,E_f,E_0)$ and $H_n(k,T,E_f)$ are computed using numerical integration techniques.

Numerical Results and Discussion

As can be seen from the preceding equations, accurate determination of the Seebeck coefficient S requires evaluation of the integral given in Eq. (5). However, due to the mathematical complexity introduced by the Gaussian distribution and Fermi–Dirac statistics, obtaining a general closed-form analytical solution for the integral in Eq. (5) remains a significant challenge. In the present study, Eq. (5) was evaluated both analytically, using the derived expression in Eq. (7), and numerically, using the Mathematica 10.0 software package. A numerical integration technique was employed to compute the Seebeck coefficient accurately over a wide temperature range. Figure shows a graph of the Seebeck coefficient as a function of temperature. The results obtained from both the analytical formula in Eq. (5) and the numerical calculations are shown on the graph, which clearly illustrates the temperature-dependent behavior of the Seebeck coefficient; there isconsistency between the two methods, thus validating the reliability of the proposed approach. In Figure, the black dashed curve represents the numerically calculated Seebeck coefficient, whereas the red solid curve depicts the values derived analytically using Eq. (5), and it can be seen that there is good agreement between them. The calculations were performed based on the parameters in Eq. (6) with values of $e=1.602\times10^{-19}C,\ L^2\sim0.864\times10^{-19}\,\frac{\text{m}^2}{\text{s}},\ \tau\sim10^{-15}$ s [24], $\sigma\sim10^{-9}\ \Omega m$ a $N_0=10^{27}m^{-3}$ [15]. As shown in Figure, the desired level of precision was achieved when the series was truncated at values for the upper limit of $N=N'=30$.

Table presents the partial sums corresponding to progressively increasing upper summation limits N in Eq. (8). Higher accuracy can be readily achieved by increasing the upper-term limits in the series expansions of Eqs. (10)–(12). The dependence of the Seebeck coefficient on temperature, which arises from the thermal broadening of the Fermi–Dirac distribution and the temperature-dependent behavior of the density of states, was systematically analyzed. The results of the numerical simulations show good agreement with the analytical expression given in Eq. (5), thus validating the accuracy of the proposed approach. These results not only validate the applicability of the numerical method but also demonstrate that the proposed approach captures the essential physics governing thermoelectric transport. It also provides a practical framework for further theoretical studies or the experimental design of semiconductor-based thermoelectric devices.

Conclusion

In this study, a novel analytical expression for the Seebeck coefficient was derived using the binomial expansion theorem and the exponential series expansion. As can be seen from Figure and Table, the general analytical expressions for the Seebeck functions obtained through the applied method exhibit strong consistency with the theoretical framework of the proposed approach. This agreement confirms the validity and accuracy of the analytical methodology used to derive the Seebeck coefficients.

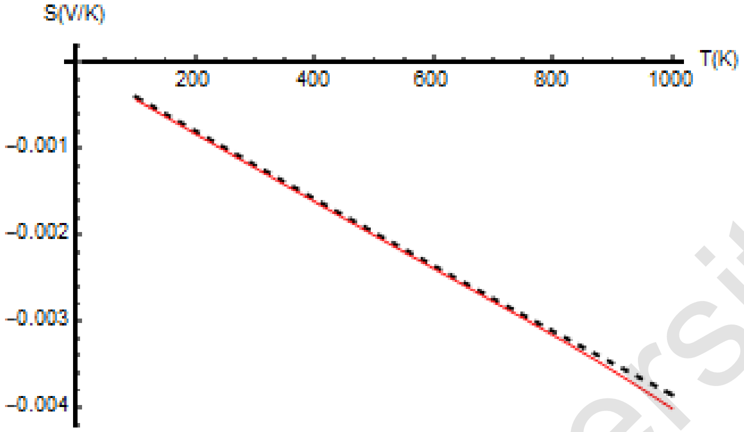

Figure. Variation in the *S* Seebeck coefficient with respect to *T* temperature (where $E_f = 2.5$ eV, $E_0 = 3.2$ eV, $k = 8.617 \times 10^{-5}$ eV $\cdot$ K^{-1}, $\delta = 1.2$ eV)

Table

Convergence of the derived expression for $Q(k, \delta, T, E_f, E_0)$ as a function of summation limits $N = N'$ (for $E_f = 8.2$ eV, $E_0 = 4.63$ eV, $k = 8.617 \times 10^{-5}$ eV $\cdot$ K^{-1}, $\delta = 1.5$ eV)

N	Eq. (5)
10	−0.000100960026019
20	−0.000101693247456
30	−0.0001018524517281
40	−0.0001019115964974
50	−0.0001019398713466
60	−0.0001019554937334
70	−0.0001019565058798

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Адам Аккуш

Ферми-Дирак жуықтауын пайдаланып Зеебек коэффициентін аналитикалық анықтауы

Зеебек коэффициенті немесе термоэлектрлік қуат — бұл материал бойынша температура градиентіне жауап ретінде пайда болатын кернеуді сандық түрде анықтайтын негізгі физикалық параметр. Бұл коэффициентті дәл анықтау термоэлектрлік құрылғылардың өнімділігін оңтайландыру үшін қажет. Зерттеуде шамамен Ферми-Дирак әдісіне негізделген жартылай өткізгіштердегі Зебек коэффициентін аналитикалық анықтауға теориялық тәсілді ұсынады. Модель Ферми деңгейінің температураға тәуелділігін ескереді, бұл тепе-теңдіксіз жылу жағдайында термоэлектрлік құрылым бойымен ішкі градиенттің пайда болуына әкеледі. Бұл модель тасымалдаушының таралуы, энергия деңгейлері мен температураның өзгеруі арасындағы өзара байланысты дәлірек түсінуге мүмкіндік береді. Алынған аналитикалық өрнектер сандық әдістердің нәтижелерімен жақсы сәйкес келеді және өнімділігі жоғары термоэлектрлік материалдарды модельдеумен жобалауда артықшылықтар береді. Ұсынылған тәсіл жартылай өткізгіш термоэлектрика саласындағы теориялық зерттеулер мен оңтайландырудың тиімді және ақпараттық құралы.

Кілт сөздер: Зеебек коэффициенті, термоэлектрлік қуат, жартылай өткізгіш, Ферми-Дирак тәсілі

Адам Аккуш

Об аналитическом определении коэффициента Зеебека с использованием приближения Ферми–Дирака

Коэффициент Зеебека или термоэлектродвижущая сила, является важным физическим параметром, который количественно описывает напряжение, возникающее в ответ на температурный градиент в материале. Точное определение этого коэффициента необходимо для оптимизации характеристик термоэлектрических устройств. В настоящем исследовании предлагается теоретический подход к аналитическому определению коэффициента Зеебека в полупроводниках на основе приближённого метода Ферми–Дирака. Модель учитывает температурную зависимость уровня Ферми, что приводит к возникновению внутреннего градиента вдоль термоэлектрической структуры в неравновесных тепловых условиях. Эта модель позволяет более точно понять взаимосвязь между распределением носителей, энергетическими уровнями и температурными изменениями. Полученные аналитические выражения хорошо согласуются с результатами численных методов и предоставляют значительные преимущества при моделировании и проектировании высокоэффективных термоэлектрических материалов. Предложенный подход является эффективным и информативным инструментом для теоретических исследований и оптимизации в области термоэлектрики полупроводников.

Ключевые слова: коэффициента Зеебека, термоэлектродвижущая сила, полупроводник, метод Ферми–Дирака

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