

Extension of the Homogeneous Electron Gas Theory to First-Order for Semiconductors with Potential Gradients

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The theory of Homogeneous Electron Gas (HEG), extensively used in solid-state and semiconductor physics, is extended to explicitly include the effect of the first-order potential gradient, whether the gradient be due to an external electric field or a gradual compositional variation. The resulting approximation is called the First-Order Homogeneous Electron Gas (FOHEG) in this work. Application of the first-order theory to the density of states shows that extra state density is introduced below the band edge by the potential gradient, a phenomenon called the Field-Induced Band Gap Narrowing (FIBGN) in this work. To study the validity of the conventional and the first-order approximations, the carrier densities are computed by both methods and compared with the exact solution to a spherical quantum dot which is so idealized that its analytic solution is available. It is found that the first-order theory better matches the exact results than the conventional one at locations beyond the classical turning point associated with the Fermi energy.

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I. Introduction

The Homogeneous Electron Gas (HEG) model of solid-state theory [1, 2] has been extensively utilized in standard semiconductor studies [3, 4]. In the HEG theory, the electrons are treated as independent particles with a constant potential energy. Since the potential energy is independent of the position, all orders of position-derivatives of the potential energy identically vanish except for the zeroth-order. Hence, the HEG can be considered as a zeroth-order theory. In the quantum mechanical treatment of this electron gas, the potential energy operator commutes with the kinetic energy operator [5].

Phenomenologically, the potential energy becomes position-dependent when an electric field or a gradual compositional variation is present in the semiconductor. Under such a circumstance, the potential energy operator and the kinetic energy operator no longer commute [5], and, rigorously speaking, the zeroth-order HEG is no longer valid either.

This article explicitly accounts for the position-dependence of the potential energy to the first-order. To be more precise, the first-order potential gradient of the semiconductor, be it due to an external field or compositional variation, is explicitly taken into account, leading to an approximation called the First-Order Homogeneous Electron Gas (FOHEG) in this work.

In Section II, the FOHEG is introduced, and the expressions for the state density and the carrier density are derived. The details of several important steps of the derivation are given in Appendices A, B, and C. In Section III, the FOHEG is shown to reduce to the HEG as the electric field approaches zero. In Section IV, the results of the approximations are given in two parts. First, the state densities of the FOHEG and the HEG are computed. Second, to study the validity of the approximations, the carrier density obtained by both methods are compared with the exact solution to a spherical quantum dot which is so idealized that it is simply like a three-dimensional simple harmonic oscillator. Finally, this article is concluded by Section V.

II. First-order homogeneous electron gas

In the theory of a homogeneous electron gas, the electrons are treated as independent particles and individually satisfy the Schrödinger equation,

$$\hat{H}\hat{A}_i(\mathbf{r}) = \epsilon_i \hat{A}_i(\mathbf{r}) \quad \text{with} \quad \hat{H} = \hat{T} + \hat{V}; \quad (1)$$

where \hat{H} is the Hamiltonian, $\hat{T} = \frac{\hat{p}^2}{2m}$ and \hat{V} are the kinetic energy and the potential energy operators, respectively, and $\hat{A}_i(\mathbf{r})$ and ϵ_i are, respectively, the eigenfunction and the eigenenergy. The eigenfunction is normalized by $\int \hat{A}_i^*(\mathbf{r})\hat{A}_i(\mathbf{r})d^3\mathbf{r} = 1$.

The carrier concentration can be calculated by solving Eq. (1) and summing over all of the probability density functions weighted by the Fermi-Dirac distribution,

$$n(\mathbf{r}) = 2 \sum_i \int |\hat{A}_i(\mathbf{r})|^2 f(\epsilon_i); \quad (2)$$

where

$$f(\epsilon) = \frac{1}{1 + e^{-(\epsilon - \epsilon_F)/kT}} \quad (3)$$

is the Fermi-Dirac distribution, $kT = 1/kT$, and ϵ_F is the Fermi level of the system. The factor of 2 in Eq. (2) is due to electron spin.

If the Non-Local Density of States (NLDS) of the electron,

$$D(\mathbf{r}; \mathbf{r}^0; \epsilon) = 2 \sum_i \pm (\hat{A}_i(\mathbf{r}) \hat{A}_i^*(\mathbf{r}^0)) \delta(\epsilon - \epsilon_i); \quad (4)$$

is introduced [6], the carrier density can be calculated by integrating over energy the product of the Local Density of States (LDS) and the Fermi-Dirac distribution,

$$n(\mathbf{r}) = \int d\epsilon D(\mathbf{r}; \mathbf{r}; \epsilon) f(\epsilon); \quad (5)$$

where the LDS is given by

$$D(\mathbf{r}; \mathbf{r}) = \lim_{\mathbf{r}^0 \rightarrow \mathbf{r}} D(\mathbf{r}; \mathbf{r}^0; \epsilon); \quad (6)$$

The NLDS in Eq. (4) can be rewritten as a \pm -operator acting on a \pm -function [7],

$$D(\mathbf{r}; \mathbf{r}^0; \pm) = 2 \pm \int \frac{d^3 \mathbf{p}}{(2\pi\hbar)^3} \frac{1}{2} (\hat{H}_{\mathbf{r}} + \hat{H}_{\mathbf{r}^0}^{\pm}) \pm(\mathbf{r}; \mathbf{r}^0); \tag{7}$$

where $\hat{H}_{\mathbf{r}}$ and $\hat{H}_{\mathbf{r}^0}^{\pm}$ are the Hamiltonian and the adjoint of the Hamiltonian operating on the \mathbf{r} - and \mathbf{r}^0 -coordinates, respectively. The completeness relation, $\int \delta(\mathbf{r} - \mathbf{r}^0) \pm(\mathbf{r}; \mathbf{r}^0) = \pm(\mathbf{r}; \mathbf{r}^0)$, has been utilized in deriving Eq. (7).

Invoking the integral representation of a delta function, the NLDS in Eq. (7) can be expressed as

$$D(\mathbf{r}; \mathbf{r}^0; \pm) = 2 \int \frac{d^3 \mathbf{p}}{(2\pi\hbar)^3} \int \frac{d\mathbf{l}}{2\pi} e^{i\mathbf{l} \cdot \mathbf{r}} e^{i\frac{1}{2}(\hat{H}_{\mathbf{r}} + \hat{H}_{\mathbf{r}^0}^{\pm})} e^{i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}^0)}; \tag{8}$$

The integrand of Eq. (8) can be expanded by using the following formula, derived in Appendix A and Ref. [7],

$$e^{i\hat{H} e^{i\mathbf{p} \cdot \mathbf{r}}} = e^{i\mathbf{p} \cdot \mathbf{r}} e^{-\frac{\mathbf{p}^2}{2m}} e^{i\frac{\hat{\mathbf{p}}^2}{2m} + \frac{\mathbf{p} \cdot \hat{\mathbf{p}}}{m} + V(\mathbf{r})}; \tag{9}$$

where $\hat{\mathbf{p}}$ is the momentum operator, and \mathbf{p} and \mathbf{r} are the momentum and position vectors, respectively. Following the treatment in Ref. [7], the exact NLDS can be further expressed as

$$\begin{aligned} D(\mathbf{r}; \mathbf{r}^0; \pm) = & 2 \int \frac{d^3 \mathbf{p}}{(2\pi\hbar)^3} \int \frac{d\mathbf{l}}{2\pi} e^{i\mathbf{l} \cdot \mathbf{r}} e^{i\frac{\mathbf{p}^2}{2m} + i\frac{1}{2}(V + V^0)} e^{i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}^0)} \\ & \exp \left[i\frac{\mathbf{l} \cdot \mathbf{p}}{2} + \frac{1}{2m} \hat{\mathbf{p}}^2 + \frac{1}{2m} \mathbf{p}^0 \cdot \hat{\mathbf{p}} + \frac{\mathbf{p}}{m} \cdot (\hat{\mathbf{p}} \cdot \mathbf{p}^0) \right. \\ & \left. + i\frac{\mathbf{l} \cdot \mathbf{p}^0}{4} + \frac{1}{2m} \hat{\mathbf{p}}^2 V + \mathbf{p}^0 \cdot \hat{\mathbf{p}} V + \frac{1}{m} \hat{\mathbf{p}} V \cdot \mathbf{p} + \mathbf{p}^0 V \cdot \mathbf{p}^0 \right. \\ & \left. + \frac{\mathbf{p}}{m} \cdot (\hat{\mathbf{p}} V \cdot \mathbf{p}^0) + \frac{i\hbar}{16m} (\hat{\mathbf{p}} V)^2 + (\mathbf{p}^0 V^0)^2 \right]; \tag{10} \end{aligned}$$

where $\hat{\mathbf{p}}$ and \mathbf{p}^0 operate on the \mathbf{r} - and \mathbf{r}^0 -coordinates, respectively, and $V = V(\mathbf{r})$ and $V^0 = V(\mathbf{r}^0)$. The Hermiticity of the Hamiltonian, $\hat{H}_{\mathbf{r}^0}^{\pm} = \hat{H}_{\mathbf{r}^0}$, has been used in deriving Eq. (10). This integral is very difficult, if not impossible, to evaluate unless the simplifying assumption is made that only algebraic terms with first order gradient of V are retained. The approximate NLDS is, thus, obtained,

$$\begin{aligned} D(\mathbf{r}; \mathbf{r}^0; \pm) \approx & 2 \int \frac{d^3 \mathbf{p}}{(2\pi\hbar)^3} \int \frac{d\mathbf{l}}{2\pi} \\ & e^{i\mathbf{l} \cdot \mathbf{r}} e^{i\frac{\mathbf{p}^2}{2m} + i\frac{1}{2}(V + V^0)} + \frac{i\hbar}{8m} \mathbf{p} \cdot (\mathbf{r} - \mathbf{r}^0) \cdot \nabla V + \frac{i\hbar}{48m} [(r_{\mathbf{r}} V)^2 + (r_{\mathbf{r}^0} V^0)^2] + i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}^0); \tag{11} \end{aligned}$$

The approximate LDS, then, follows by letting $r^0 = r$ as in Eq. (6),

$$D(F; r) \approx \frac{1}{2} \int \frac{d^3 p}{(2\pi)^3} e^{i \left[\frac{p^2}{2m} + V(r) \right]} \left(\frac{1}{24m} \right)^2 (rV)^2; \quad (12)$$

This approximation only retains the first-order derivative terms of the potential energy, and is called the First-Order Homogeneous Electron Gas (FOHEG) theory in this work. Note that Eq. (12) can also be derived by retaining higher order commutator relations, this alternative derivation is given in Appendix B.

The integral over p in Eq. (12) can be performed with the formula

$$\int \frac{d^3 p}{(2\pi)^3} e^{i \frac{p^2}{2m}} = \frac{m}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{t^2} dt; \quad (13)$$

and the LDS in Eq. (12) is evaluated to be

$$D(F; r) = \frac{1}{4} \frac{m}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{t^2} dt e^{i \left[\frac{p^2}{2m} + V(r) \right]} e^{i a^3 t^3}; \quad (14)$$

with $a^3 = \frac{-2(rV)^2}{24m}$.

For further evaluation of Eq. (14), the Fourier representation of [8, 9]

$$e^{i a^3 t^3} = \int_{-\infty}^{\infty} dt Ai(t) e^{i b^3 t} \quad \text{with } b^3 = 3a^3; \quad (15)$$

and the complex integral of [10],

$$\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{t^2} dt e^{i \mu t} = \frac{1}{4} \mu^{1/2} \mu^{(0)}; \quad (16)$$

are utilized, where Ai and γ are, respectively, the Airy and gamma functions as defined in Ref. [11], μ is the unit step function, and the derivation of Eq. (15) is given in Appendix C. The LDS in Eq. (14), thus, results in a rather compact form,

$$D(F; r) = \frac{4}{\pi} \frac{m}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{t^2} b^{1/2} \int_{-\infty}^{\infty} dt Ai(t) (t + \eta)^{1/2}; \quad (17)$$

where $b^3 = 3a^3 = \frac{-2(rV)^2}{8m}$, and $\eta = \frac{\eta_i V}{b}$. A one-fold numerical integration needs to be performed to evaluate the LDS.

Once the LDS is obtained, the carrier density follows directly from Eq. (5),

$$n(r) = \frac{4}{\pi} \frac{\mu}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{t^2} \int_{-\infty}^{\infty} dt Ai(t) (t + \eta)^{1/2} f(\eta); \quad (18)$$

where

$$f(\eta) = \frac{1}{1 + e^{-\eta}} \quad (19)$$

is the Fermi-Dirac distribution in normalized quantities, $\eta = \frac{b}{kT}$, $\mu = \frac{V_i}{b}$, and $\eta_F = \frac{V_i}{b}$. Note that $\eta(\mu; \eta_F) = \eta(\mu; \eta_F)$. A two-fold numerical integration has to be performed for the evaluation of the carrier density given by Eq. (18).

III. Relations to homogeneous electron gas theory

In this section, it will be shown that the first-order homogeneous electron gas theory of this work reduces to the homogeneous electron gas theory as the electric field gradually diminishes. Specifically, it will be demonstrated that the LDS in Eq. (17) and the carrier density in Eq. (18) approach the results of the homogeneous electron gas as the electric field vanishes.

If $j_r V_j \neq 0$, then $b \neq 0^+$, and the analysis of the limiting behavior of the LDS in Eq. (17) is divided into two cases, depending on the sign of $(\mu; V)$.

First, suppose that $(\mu; V) > 0$. As $j_r V_j \neq 0$, $b \neq 0^+$, then $\eta \neq 1$ and $b\eta = \mu; V$. Equation (17) is rewritten as

$$\begin{aligned} D(\mathcal{F}; \mu) &= \frac{4}{\pi^{3/4}} \frac{m}{2^{3/4} \hbar^2} \int_0^{\infty} dt A_i(t) (bt + \mu; V)^{1/2} \\ &= \frac{4}{\pi^{3/4}} \frac{m}{2^{3/4} \hbar^2} (\mu; V)^{1/2}; \end{aligned} \quad (20)$$

where the integral of $A_i(t)$ is identified to be 1 because it is known from Ref. [11] that $\int_0^{\infty} dt A_i(t) = \frac{1}{2} \int_0^{\infty} dt A_i(t) = \frac{1}{3}$.

Second, suppose that $(\mu; V) < 0$. As $j_r V_j \neq 0$, $b \neq 0^+$, then $\eta \neq 1$. The integration interval diminishes. Hence, $D(\mathcal{F}; \mu) \neq 0$.

Conclusively, as $j_r V_j \neq 0$, $b \neq 0^+$, the LDS in Eq. (17) reduces to

$$D(\mathcal{F}; \mu) = \frac{4}{\pi^{3/4}} \frac{m}{2^{3/4} \hbar^2} (\mu; V)^{1/2} \mu(\mu; V) \quad \text{if } j_r V_j \neq 0; \quad (21)$$

which is the density of states of the homogeneous electron gas in standard semiconductor physics textbooks [3, 4].

The carrier density at the low-field limit, therefore, follows from Eq. (5),

$$n(\mathcal{F}) = 2 \frac{\mu}{2^{3/4} \hbar^2} \int_0^{\infty} F_{1/2} \left(\frac{\mu; V_i}{kT} \right) \quad \text{if } j_r V_j \neq 0; \quad (22)$$

where

$$F_j(x) = \frac{1}{\Gamma(j+1)} \int_0^{\infty} dt \frac{t^j}{1 + e^{t+x}} \quad (23)$$

is the Fermi-Dirac integral of order j and argument x [12]. For non-degenerate semiconductors, $(V_i; \eta_F) > 3kT$, the carrier density given in Eq. (22) further reduces to

$$n(\mathcal{F}) = 2 \frac{\mu}{2^{3/4} \hbar^2} \exp \left(\frac{\mu; V_i}{kT} \right); \quad (24)$$

Equation (24) indeed is the carrier density of the homogeneous electron gas, and is frequently used in elementary semiconductor textbooks [3, 4].

Moreover, the carrier density of a system with very large Fermi energy, $\mu_F \gg V$, can be shown to reduce to the classical limit of free-electron gas by the following arguments.

Because of the Fermi-Dirac distribution function, the integrand of the carrier density integral given by Eq. (18) is negligibly small if μ is a few kT larger than μ_F . Hence, when the Fermi level is large, negligible error is introduced into the integral by the approximation where the LDS is approximated by Eq. (21), and the Fermi-Dirac distribution is approximated by a unit step function. The carrier density is, then, evaluated to be

$$n(\mu) = \frac{8}{3\pi^{3/2}} \frac{m(\mu_F - V)^{3/2}}{2^{3/2}} \quad (25)$$

This is the classical limit of the first-order theory. Noting that Eq. (25) involves no potential gradient, the carrier density is independent of the applied electric field if the Fermi level is far above the conduction-band edge, and can be re-expressed in a more popular form,

$$n(\mu) = \frac{k_F^3}{3\pi^2} \quad \text{with} \quad k_F = \frac{2m(\mu_F - V)^{1/2}}{\hbar} \quad (26)$$

which is the carrier density of the free-electron gas given in solid-state textbooks [1].

Therefore, it is shown in this section that the homogeneous electron gas is the low-field limit of the first-order homogeneous electron gas of this work, and that the first-order theory reduces to the classical limit of the free-electron gas at large Fermi energy.

IV. Results and discussions

In contrast to the conventional Homogeneous Electron Gas (HEG) theory, the First-Order Homogeneous Electron Gas (FOHEG) theory of this work explicitly takes the potential gradient into account. The potential gradient effects will be illustrated in this section by comparing the Local Density of States (LDS or simply DOS) and the carrier density obtained by both methods.

The DOS's obtained by the FOHEG in Eq. (17) and by the HEG in Eq. (21) are plotted in Fig. 1 by solid and dashed lines, respectively. In this plot, the DOS is normalized by $(4\pi)^{-1/2} (m/2\pi\hbar^2)^{3/2} b^{1/2}$, and the normalized energy scale is $\epsilon = (\mu - V)/b$ with $b^3 = \hbar^2 |r| V^2 / 8m$. Comparison of the DOS's calculated by the FOHEG and the HEG shows two features. First, the potential gradient causes the waviness of the DOS curve. And the waviness gradually diminishes as the normalized energy increases, indicating that the effect decreases with increasing energy. Second, at energies below the band edge ($\mu < V$ or $\epsilon < 0$), the HEG predicts vanishing DOS, whereas, the FOHEG shows that the potential gradient introduces states in the forbidden band gap predicted by the flat-band theory. These induced states are due to quantum tunneling of wave functions beyond the classical turning point. The tunneling effectively lowers the conduction band edge and reduces the band gap, leading to a phenomenon called the Field-Induced Band Gap Narrowing (FIBGN) in this work. Obviously, explicit negligence of the potential gradient in the conventional theory can not account for this tunneling effect.

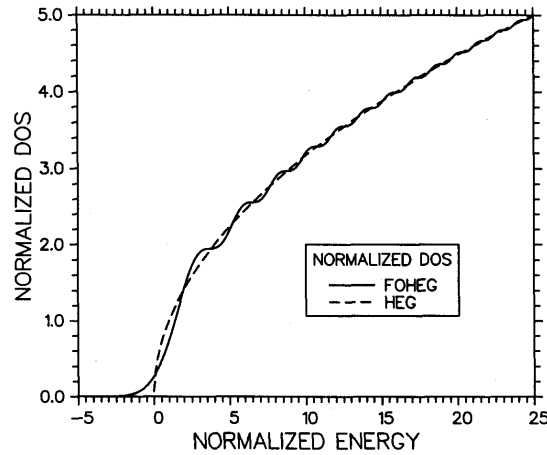


FIG. 1. The normalized density of states is plotted as a function of the normalized energy ($\epsilon = (\epsilon_i - V)/b$). The DOS's predicted by the FOHEG and by the HEG are sketched by solid and dashed lines, respectively.

In order to study the validity of the FOHEG and the HEG, the carrier densities obtained by both approximations are computed and compared for systems with analytic solutions. The exact solution to an ideal spherical quantum dot with the confinement potential of

$$V(r) = \frac{1}{2}m\omega^2 r^2 \quad (27)$$

is used as a test vehicle, where m , ω , and r are the effective mass, the angular frequency, and the radial distance from the origin, respectively.

In this article, the ideal quantum dot is hypothetical and is assumed to be manufactured by continually changing the composition x of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ crystal from 0 to 0.4 in the radial direction. Since $\text{Al}_x\text{Ga}_{1-x}\text{As}$ with $x < 0.4$ is a direct-band material, and the conduction band edge difference between $\text{Al}_{0.4}\text{Ga}_{0.6}\text{As}$ and GaAs is about 0.448 eV, the angular frequency of the ideal spherical quantum dot is taken so that $\hbar\omega = 35.8857$ meV in order to have enough quantum levels within the confinement potential.

If the compositional dependence of the effective mass of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ is ignored, the ideal quantum dot is essentially a three-dimensional Simple Harmonic Oscillator (SHO) with the eigen-energy of

$$E_n = \hbar\omega \left(n + \frac{3}{2} \right) \quad (28)$$

where $n = 0; 1; 2; \dots$, and $n = 0$ corresponds to the ground state. The GaAs effective mass of $m = 0.067 m_0$ is assumed in the rest of the computation, where m_0 is the electron rest mass.

The carrier densities obtained by the exact solution, the FOHEG, and the HEG approximations to the above hypothetical quantum dot are plotted in Fig. 2 by solid, dashed, and dotted lines, respectively, for Fermi energies at $\mu = 0.1$ eV, the zeroth ($E_0 = 5.3829 \times 10^{-2}$ eV, ground level), the fourth ($E_4 = 1.9737 \times 10^{-1}$ eV), and the tenth ($E_{10} = 4.1269 \times 10^{-1}$ eV) quantum

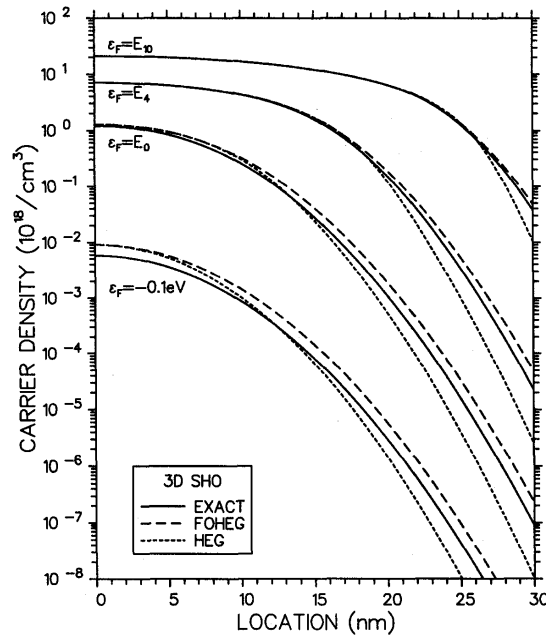


FIG. 2. The carrier densities of a three-dimensional SHO are plotted as functions of location for Fermi energies at μ 0.1 eV, the zeroth ($E_0 = 5.3829 \times 10^{i-2}$ eV, ground level), the fourth ($E_4 = 1.9737 \times 10^{i-1}$ eV), and the tenth ($E_{10} = 4.1269 \times 10^{i-1}$ eV) quantum levels of the SHO. The carrier densities obtained by the exact solution, the FOHEG, and the HEG are drawn by solid, dashed, and dotted lines, respectively.

levels of the SHO. Three features are observed in the figure. First, both the FOHEG and the HEG deviate from the exact solution at low Fermi energies (for instance, $\mu_F = \mu$ 0.1 eV and E_0). There must be a large enough number of quantum levels below the Fermi level for the FOHEG prediction to sufficiently approach the exact solution (for instance, $\mu_F = E_4$ and E_{10}). Second, comparison of the FOHEG results with successively higher Fermi levels ($\mu_F = E_0$; E_4 , and E_{10}) shows that systems with more quantum levels below the Fermi level better approach the exact solution, demonstrating the statistical nature of the approximation. Third, at radial locations exceeding the classical turning point associated with the Fermi energy, $r_F = \sqrt{2\mu_F/m}$, the HEG starts to deviate from the exact solution more significantly; whereas, the FOHEG better matches the exact results. This is due to the fact that the tunneling effects of the wave functions beyond the classical turning point is included in the formulation of FOHEG as illustrated in Fig. 1.

V. Conclusions

In this article, the Homogeneous Electron Gas (HEG) theory in the literature is extended to include the effects of the first-order derivative of the potential energy. This approximation is called the First-Order Homogeneous Electron Gas (FOHEG) theory in this work, and is applicable to bulk semiconductors with band-bending.

The state density and the carrier density obtained by the FOHEG theory are expressed by formulae given by Eqs. (17) and (18), respectively. These expressions reduce to the flat-band equations frequently encountered in standard textbooks when the electric field approaches zero.

The density of states is computed and compared with the results of the homogeneous electron gas. It is found that, because of the tunneling of wave functions beyond the classical turning point, the electric field introduces states in the forbidden band gap of the homogeneous electron gas. Hence, the conduction band edge is effectively lowered, and the band gap is accordingly narrowed, a phenomenon called the Field-Induced Band Gap Narrowing (FIBGN) in this work.

To study the validity of the FOHEG and the HEG theory, both approximations are used to calculate the carrier density of an ideal spherical quantum dot. The spherical quantum dot is so idealized that it is essentially a three-dimensional simple harmonic oscillator, which provides a case with exact solutions for comparison with the approximate methods.

Because of the statistical nature of the approximation, the FOHEG results better match the exact solution for systems with more quantum levels below the Fermi level. Moreover, at location exceeding the classical turning point, the carrier density predicted by the FOHEG theory matches better the exact result than the conventional HEG theory because the FOHEG includes the tunneling effects over the turning point.

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Appendix A: Derivation of Equation (9)

Although Eq. (9) had been derived in Ref. [7], a more transparent derivation based on matrix mechanics [5] is given in this appendix.

The displacement operator in the momentum space is given by $T(\mathfrak{p}) = e^{i\mathfrak{p}\hat{q}}$, where \mathfrak{p} is the momentum displacement and \hat{q} is the position operator. The momentum displacement operator, $T(\mathfrak{p})$, is unitary, namely, it satisfies $T(\mathfrak{p})^\dagger T(\mathfrak{p}) = T(\mathfrak{p})T(\mathfrak{p})^\dagger = \hat{1}$. The translation in momentum space is, thus, $T(\mathfrak{p})^\dagger \hat{p} T(\mathfrak{p}) = \hat{p} + \mathfrak{p}$, where \hat{p} is the momentum operator.

Application of the momentum translation operator to the Hamiltonian given in Eq. (1) yields,

$$T(\mathfrak{p})^\dagger \hat{H} T(\mathfrak{p}) = \frac{(\hat{p} + \mathfrak{p})^2}{2m} + V(\hat{q}) \quad (\text{A1})$$

Therefore, the momentum translation operator acting on $e^{-\hat{H}}$ gives,

$$T(\mathfrak{p})^\dagger e^{-\hat{H}} T(\mathfrak{p}) = e^{i\mathfrak{p}\hat{q}} e^{-\hat{H}} e^{-i\mathfrak{p}\hat{q}} = e^{-\frac{(\hat{p} + \mathfrak{p})^2}{2m} + V(\hat{q})} = e^{-\frac{\hat{p}^2}{2m}} e^{-\frac{\mathfrak{p}\hat{p}}{m} + V(\hat{q})} \quad (\text{A2})$$

Equation (9) follows immediately from Eq. (A2) if the position representation of the above operator equation is taken.

Appendix B: Alternative derivation of Equation (12)

It was shown in Ref. [7] that

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} \mathbb{1}_0 \exp \int_0^1 d\alpha e^{\alpha \hat{A}} \hat{B} e^{-\alpha \hat{A}}; \quad (\text{B1})$$

where α is a parameter varying from 0 to 1, $d\alpha$ is the infinitesimal differential of α , and $\mathbb{1}_0$ represents the product of the infinitesimal exponential operator behind it. Note that

$$e^{\alpha \hat{A}} \hat{B} e^{-\alpha \hat{A}} = \sum_{n=0}^{\infty} \frac{(\alpha \hat{A})^n}{n!} [\hat{B}; \hat{A}]^n; \quad (\text{B2})$$

and

$$[\hat{A}]^n \hat{B} = [[\hat{B}; \hat{A}]; \hat{A}]^n; \quad (\text{B3})$$

where the operator \hat{A} appears n times on the right-hand side of Eq. (B3).

From Eqs. (B1) to (B3), the approximation to $e^{\hat{A}+\hat{B}}$ can be obtained as follows. Suppose that $[\hat{A}; \hat{B}] \neq 0$ and $[[\hat{A}; \hat{B}]; \hat{A}] \neq 0$, but $[[\hat{A}; \hat{B}]; \hat{B}] = 0$ and $[[[\hat{A}; \hat{B}]; \hat{A}]; \hat{A}] = [[[\hat{A}; \hat{B}]; \hat{A}]; \hat{B}] = 0$. Then the first three terms of Eq. (B2) are non-vanishing. And the following formula is obtained,

$$e^{\hat{A}+\hat{B}} = e^{i \frac{1}{2} [[\hat{A}; \hat{B}]; \hat{A}]} e^{\hat{A}} e^{i \frac{1}{2} [[\hat{A}; \hat{B}]; \hat{B}]}; \quad (\text{B4})$$

Only one of the two second-order commutators is retained in the supposition.

Operators \hat{A} and \hat{B} are substituted by $i \frac{1}{2} \hat{V}$ and $i \frac{1}{2} \hat{T}$, respectively. It can be shown that the commutator equalities and inequalities in the suppositions of the second order approximation are either exactly or approximately satisfied if the second- and higher-order derivatives of V are ignored. In particular, the two non-vanishing identities are given by

$$[\hat{V}; \hat{T}] \approx \frac{i}{m} r \cdot \nabla \hat{p}; \quad (\text{B5})$$

and

$$[[\hat{V}; \hat{T}]; \hat{V}] = \frac{\hbar^2}{m} (r \cdot \nabla \hat{p} \cdot \nabla); \quad (\text{B6})$$

Substituting the approximations in Eqs. (B5) and (B6) into Eq. (B4), it follows that

$$e^{i \frac{1}{2} \hat{H}} = e^{i \frac{1}{2} (\hat{V} + \hat{T})} \frac{1}{4} e^{i \frac{2 \hbar^2}{48m} (r \cdot \nabla)^2} e^{i \frac{1}{2} \hat{V}} e^{i \frac{1}{8m} r \cdot \nabla \hat{p}} e^{i \frac{1}{4m} \hat{p}^2}; \quad (\text{B7})$$

When the above exponential Hamiltonian operator acts on a plane wave, the following approximate equation emerges,

$$e^{i \frac{1}{2} \hat{H}} e^{i \mathbf{p} \cdot \mathbf{r}} \approx \frac{1}{4} e^{i \frac{1}{2} (V + \frac{p^2}{2m})} e^{i \frac{1}{8m} r \cdot \nabla \hat{p}} e^{i \frac{2 \hbar^2}{48m} (r \cdot \nabla)^2} e^{i \mathbf{p} \cdot \mathbf{r}}; \quad (\text{B8})$$

Substituting Eq. (B8) into Eq. (8), and noting the Hermiticity of the Hamiltonian, the NLDS in Eq. (11) and the LDS in Eq. (12) are rederived.

Appendix C: Derivation of Equation (15)

In this appendix, the function $e^{i a^3 t^3}$ is shown to be the Fourier transformation of the Airy function by using its integral representation given in Refs. [7-9],

$$e^{i a^3 t^3} = \frac{2}{3} \int_0^{\infty} dt \left(J_{\frac{1}{3}}(2t) + J_{-\frac{1}{3}}(2t) \right) e^{i t^3} + \frac{\rho_{\frac{1}{3}}}{\frac{1}{4}} K_{\frac{1}{3}}(2t) e^{i t^3}; \quad (C1)$$

where J and K are the Bessel functions. Observing the relations between Bessel functions and Airy function, Ai, given by Ref. [11],

$$J_{\frac{1}{3}}(2t) + J_{-\frac{1}{3}}(2t) = \frac{1}{(3t)^{\frac{1}{3}}} \text{Ai} \left((3t)^{\frac{2}{3}} \right) \quad (C2)$$

and

$$K_{\frac{1}{3}}(2t) = \frac{\rho_{\frac{1}{3}}}{(3t)^{\frac{1}{3}}} \text{Ai} \left((3t)^{\frac{2}{3}} \right); \quad (C3)$$

Eq. (15) is obtained by changing variables $t = (3t)^{\frac{2}{3}}$.

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