New Scaling of Child-Langmuir Law in the Quantum Regime

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This paper presents a consistent quantum mechanical model of Child-Langmuir (CL) law, including electron exchange-correlation interaction, electrode's surface curvature, and finite emitter area. The classical value of the CL law is increased by a larger factor due to the electron tunneling through the space-charge potential, and the electron exchange-correlation interaction becomes important when the applied gap voltage V_g and the gap spacing D are, respectively, on the order of Hartree energy level, and nanometer scale. It is found that the classical scaling of $V_g^{3/2}$ and D^{-2} is no longer valid in the quantum regime, and a new scaling of $V_g^{1/2}$ and D^{-4} is established. The smooth transition from the classical regime to the quantum regime is also demonstrated.

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The classical Child-Langmuir (CL) law [1] gives the maximum current density allowed for steady-state electron beam transport across a gap of gap spacing D and gap voltage V_g. In the one-dimensional (1D) planar, and nonrelativistic model (with zero electron emission energy), the classical 1D CL law is

$$J_{\mathrm{CL}} = \frac{4\epsilon_0}{9}\sqrt{\frac{2e}{m}}\frac{V_g^{3/2}}{D^2}, \tag{1}$$

where e and m are the charge and mass of the electron, respectively, and ϵ_0 is the free space permittivity. From the equation, the classical scaling of the limiting current density J_{CL} to the 3/2's power of gap voltage ($J_{\mathrm{CL}} \propto V_g^{3/2}$), and to the inverse squared power of gap spacing ($J_{\mathrm{CL}} \propto D^{-2}$), is widely used in the fields of high-current emission diodes, vacuum microelectronics, high power microwave sources, accelerator physics, and sheath physics. While Eq. (1) is easy to derive, it was only recently that the 1D classical CL law was extended to a two-dimensional (2D) model with simulation results [2], and with analytical solutions [3]. The effects of nonuniform current emission [4] from a finite emitter area and of the current's short pulse [5] have also been studied. Recent developments of the multidimensional CL law in classical regime can be found in a review paper [6].

In the emerging fields of nanotechnology, nanostructures such as nanodiodes, nanotriodes, and nanogaps ranging from sub-10 nm to 100's of nm are readily fabricated [7–9]. In such a nanometer scale, it is of interest to study the intense beam-gap interaction, such as the limiting current density (or CL law) for a nanosized gap, where quantum effects are important. However, compared to the classical models [1–6], there are relatively few investigations of CL law in the quantum regime [10,11]. In the 1D quantum models, mean field theory has been used to calculate the CL current density by assuming that the electron density in the gap is high enough to include only the electron space-charge field, but not for the electron quantum interaction (the exclusion principle is ignored) [10,11]. This assumption is clearly not valid when the electron's energy scale is comparable to the Hartree energy, in which case the electron exchange-correlation interaction cannot be ignored.

Thus, in this context, several interesting questions arise: Is the electron exchange-correlation interaction important for a wide range of gap voltage and gap spacing? Are the classical scaling of $V_g^{3/2}$ and D^{-2} valid in the quantum regime? What are the equivalent cylindrical and spherical CL laws in the quantum regime? How does one derive a simple 2D quantum CL law? This Letter addresses these questions.

Consider electrons with emission energy E (with respect to Fermi energy, E_F) injected normally into a nanosize gap with a gap spacing D, where the emitter ($x = r_k$) is grounded, and the collector ($x = r_k + D$) is held at a dc voltage V_g. Using mean field theory, we solve the time-independent Schrödinger equation, the Poisson equation, and the charge conservation relation to obtain the mean electron density profile inside the gap for a given current density J. From the calculated density profile, we use the Kohn-Sham density functional theory [12] to calculate the electron exchange-correlation potential (in terms of the Hartree energy E_H):

$$V_{\mathrm{xc}} = \epsilon_{\mathrm{xc}} - \frac{r_S}{3}\frac{d\epsilon_{\mathrm{xc}}}{dr_S}, \tag{2}$$

where r_S is the local Seitz radius ($4\pi n r_S^3/3 = 1$), in terms of the Bohr radius a_0. Here, the $\epsilon_{\mathrm{xc}} = \epsilon_x + \epsilon_c$ is the exchange-correlation energy per particle for a uniform electron gas of density n, under the Kohn-Sham local density approximation (LDA), where ϵ_x is the exchange energy contribution [13] and ϵ_c is the correlation energy

contribution [14]. They are

$$\epsilon_x = -\frac{3}{4}\left(\frac{3}{2\pi}\right)^{2/3}\frac{1}{r_S}, \tag{3a}$$

$$\epsilon_c = -2A(1 + a_1 r_S)\ln\left[1 + \frac{1/2A}{\kappa}\right], \tag{3b}$$

where $\kappa = b_1\sqrt{r_S} + b_2 r_S + b_3 r_S^{3/2} + b_4 r_S^{c+1}$, and $(c, A, a_1, b_1, b_2, b_3, b_4)$ are parametrized constants under random phase approximation [15].

For convenience, we introduce the normalized parameters: $\bar{x} = x/D$, $\phi = V/V_g$, $\lambda = D/\lambda_0$ is the normalized gap spacing, $\phi_g = eV_g/E_H$ is the normalized gap voltage, $\epsilon = (E - E_F)/eV_g$ is the normalized electron emission energy, and $q^2 = n/n_0 = |\psi|^2/n_0$ is the normalized electron density. The normalized scales $\lambda_0 = \sqrt{\hbar^2/2emV_g}$ is the electron de Broglie wavelength at V_g, $n_0 = 2\epsilon_0 V_g/3eD^2$ is the density scale, $E_H = e^2/4\pi\epsilon_0 a_0 = 27.2\,\mathrm{eV}$ is the Hartree energy, and $a_0 = 4\pi\epsilon_0\hbar^2/me^2 = 0.0529\,\mathrm{nm}$ is the Bohr radius.

For a given gap spacing D and gap voltage V_g, λ measures the ratio of gap spacing to the electron de Broglie wavelength, and ϕ_g measures the ratio of gap voltage to the Hartree energy, where $\lambda \gg 1$ and $\phi_g \gg 1$ are the classical limits. In terms of the normalized parameters, the time-independent Schrödinger equation, the Poisson equation, and the charge conservation relation can be rewritten into a two-coupled nonlinear equation of $q(\bar{x})$ and $\phi(\bar{x})$:

$$q'' + \frac{N}{\bar{x}}q' + \lambda^2\left[\epsilon + \phi - \phi_{\mathrm{xc}} - \frac{4}{9}\frac{\mu^2[N]R^{2N}}{\bar{x}^{2N}q^4}\right]q = 0, \tag{4}$$

$$\phi'' + \frac{N}{\bar{x}}\phi' = \frac{2}{3}q^2, \tag{5}$$

where the prime denotes the derivative with respective to $\bar{x}$. Here, $\phi_{\mathrm{xc}}(<0) \equiv \phi_x + \phi_c = V_{\mathrm{xc}}[r_S]/\phi_g$, and $V_{\mathrm{xc}}[r_S]$ is the exchange-correlation potential given in Eqs. (2) and (3), which is a function of normalized density $q^2(\bar{x})$ through the dependence of $r_S(\bar{x}) = [3\lambda/2\phi_g q(\bar{x})]^{2/3}$. In Eqs. (4) and (5), the integer $N = 0, 1, 2$ denotes three basic geometries: planar ($N = 0$), cylindrical ($N = 1$), spherical ($N = 2$); and the parameters $\mu[N]$ are, respectively, the normalized current density, normalized current line density, and normalized total current. The normalizations are $\mu[0] = J/J_{\mathrm{CL}}$, $\mu[1] = J/2\pi RDJ_{\mathrm{CL}}$, and $\mu[2] = J/4\pi R^2D^2J_{\mathrm{CL}}$, where $R = r_k/D$ measures the curvature of the gap with respect to the gap spacing D.

In deriving Eqs. (4) and (5), we have assumed that the electron wave function is of complex form $\psi = \sqrt{n_0}q(\bar{x})\exp[i\theta(\bar{x})]$, where $q(\bar{x})$ and $\theta(\bar{x}) = \frac{2}{3}\mu[N]R^N\sqrt{\lambda}\times\int_{R+1}^{\bar{x}}\bar{x}^{-N}q^{-2}(\bar{x})d\bar{x} + \theta(R+1)$ are, respectively, the normalized real functions of the wave amplitude and phase. To obtain the boundary conditions for the equations, we match the wave function ψ to a transmitted plane wave at the collector ($\bar{x} = R + 1$), where the transmitted plane wave is obtained from solving Eq. (4) at $\phi_{\mathrm{xc}} = 0$, $\mu[N] = 0$, and $\phi = \phi(R+1) = 1$. The boundary conditions for Eqs. (4) and (5) are

$$\phi(R) = 0, \tag{6a}$$

$$\phi(R+1) = 1, \tag{6b}$$

$$q(R+1) = \frac{\sqrt{2\mu[N]R^N/3}}{(1+\epsilon)^{1/4}(R+1)^{N/2}}, \tag{6c}$$

$$q'(R+1) = -(R+1)^{N/2}\xi[N]q(R+1), \tag{6d}$$

where $\xi[N] = 0$, $\eta/\sqrt{R+1}$, and $1/(R+1)^2$ for $N = 0, 1$, and 2, respectively. Here, $\eta = (J_0J_1 + Y_0Y_1)/(J_0^2 + Y_0^2)$ and J_0, J_1, Y_0, Y_1 are the Bessel functions evaluated at the argument $\bar{x} = \lambda(R+1)\sqrt{1+\epsilon}$. With the boundary conditions, we determine the quantum CL law, through the maximum value of $\mu[N]$, defined as $\mu_Q[N]$. For $\mu > \mu_Q$, solutions to Eqs. (4) and (5) no longer exist.

In the classical limit at $\lambda \gg 1$ and $\phi_g \gg 1$, Eqs. (4) and (5) become

$$\phi'' + \frac{N}{\bar{x}}\phi' = \frac{4}{9}\mu[N]\frac{R^N}{\bar{x}^N\sqrt{\epsilon + \phi}}, \tag{7}$$

which is the governing equation (independent of λ and ϕ_g) to calculate the maximum value of $\mu_Q[N] = \mu_{\mathrm{CL}}[N]$ in the classical regime. For a planar configuration ($N = 0$) at zero emission energy ($\epsilon = 0$), Eq. (7) simply gives $\mu_Q = 1$, which recovers the 1D classical CL law: $J_Q = J_{\mathrm{CL}}$ [1].

Figure 1 shows the calculated μ_Q as a function of λ for various values of ϕ_g at $\epsilon = 0$ and $N = 0$ (planar). For a given ϕ_g, μ_Q increases with decreasing values of λ(quantum regime) and exceeds the classically predicted values when $\lambda \lesssim 10$. The value of μ_Q is roughly proportional to λ^{-2} at small λ, and this indicates that $J_Q \propto D^{-4}$ is the correct scaling in the quantum regime for small D, as compared to the classical scaling of $J_{\mathrm{CL}} \propto D^{-2}$. From

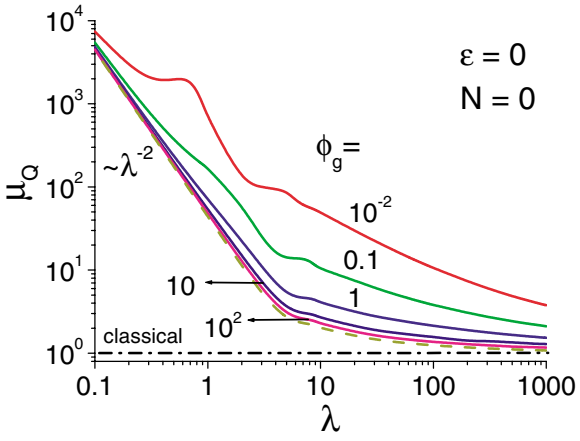

FIG. 1 (color online). The normalized quantum CL law μ_Q as a function of λ for various $\phi_g = 10^{-2}$ to 10^2 (solid lines: top to bottom), $\phi_g \gg 1$ (dashed line), and classical limit (dash-dotted line).

the figure, we also see that the enhancement of μ_Q is more dominant at small ϕ_g due to electron exchange-correlation interaction, and previous results are recovered [10,11] at $\phi_g \gg 1$ (dashed line). This last statement implies that electron exchange-correlation interaction (ϕ_{xc}) cannot be ignored at low gap voltage when it is on the order of Hartree energy level.

To investigate the scaling of limiting current to gap voltage in the quantum regime, the product of μ_Q and $V_g^{3/2}$ is plotted in Fig. 2 as a function of V_g for various values of D (solid lines). It is clear that the scaling of the limiting current density to the 3/2's power of gap voltage is no longer valid for small V_g at a fixed D, and the new scaling is $J_Q \propto V_g^{1/2}$ in the quantum regime for small V_g. The cases with no exchange-correlation interaction, $\phi_{xc} = 0$ (dashed lines), and the classical limit (short dashed line) are also plotted for comparison. The comparison proves the importance of the electron exchange-correlation interaction at small V_g and D.

According to the classical CL law, the limiting current density ($\mu_Q \geq 1$) exists only for non-negative electron emission energy ($\epsilon \geq 0$). However, there is finite probability of electron tunneling in the quantum regime for negative electron emission energy ($\epsilon < 0$). In Fig. 3(a), we show μ_Q as a function of D at $V_g = 1$ V for various values of $\epsilon = 0.5$ to -0.5. For $\epsilon < 0$, we see that $\mu_Q \rightarrow 0$ decreases sharply from the quantum regime to the classical regime with an increase of D. In Fig. 3(b), we show the boundary of the transition between the quantum and the classical regime at $E - E_F$ [eV] = -0.2, -0.3, and -0.5, where the boundary is defined as the calculated values of D at $\mu_Q = 1$ for a given gap voltage V_g. For example, at $E - E_F = -0.2$ eV, the boundaries are $D = 63$ nm and $D = 240$ nm for $V_g = 1$ V and 10 V, respectively.

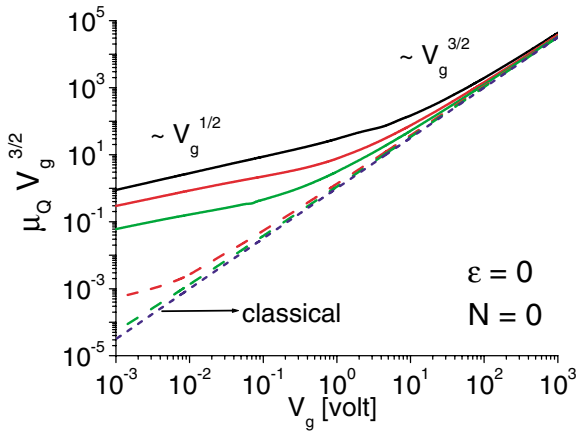

FIG. 2 (color online). The values of $\mu_Q V_g^{3/2}$ as a function of gap voltage V_g (volt) for various gap spacing $D = 1$, 10, and 100 nm (solid lines: top to bottom). The dashed lines are without an exchange-correlation term ($\phi_{xc} = 0$) for $D = 10$ and 100 nm (top to bottom), and the short-dashed line is the classical limit.

In Fig. 4(a), we show the equivalent cylindrical ($N = 1$) and spherical ($N = 2$) models of the quantum CL law for $D = 10$ nm (solid lines) and $D = 100$ nm (dashed lines) at $\epsilon = 0$ and $V_g = 1$ V. For comparison, calculations at $D = 10$ nm and $V_g = 10$ V are also plotted, which show little differences between $V_g = 1$ V and $V_g = 10$ V. From the figure, we see that the limiting current $\mu[N = 1, 2]$ (with respect to $\mu[N = 0]$) increases with small values of R, and it recovers to the planar case at $R > 100$. Note that $\mu[N = 2]$ is larger than $\mu[N = 1]$ for a given R, V_g, and D, and that at a fixed value of N the curves in Fig. 4(a) are insensitive to D and V_g over the range studied.

It has been shown recently that the 1D classical CL law can be extended analytically to a simple 2D model by using only the 1D electron density profile, and the analytical 2D classical CL law [3] agrees very well with simulation results [2]. Pretending that the same method may be applied to quantum corrections, we obtain the following expressions for μ_Q[2D]:

$$\frac{\mu_Q[2D]}{\mu_Q[1D]} = 1 + \frac{4}{\pi}\frac{D}{W}\rho, \tag{8a}$$

$$\frac{\mu_Q[2D]}{\mu_Q[1D]} = 1 + \frac{D}{R}\rho, \tag{8b}$$

$$\frac{\mu_Q[2D]}{\mu_Q[1D]} = 1 + \left[\frac{4}{\pi}\frac{D}{W} + \left(1 - \frac{2}{\pi}\right)\frac{D}{R}\right]\rho, \tag{8c}$$

for an infinitely long emitting strip of width W, a circular emitting patch of radius R, and an emitting ellipse of semiaxes R and $W/2 < R$, respectively. Here, the parameter ρ measures the mean position of the electrons in the gap, and it is a function of λ and ϕ_g, defined as $\rho(\lambda, \phi_g) = \int_0^1 \bar{x} q^2(\bar{x}) d\bar{x} / \int_0^1 q^2(\bar{x}) d\bar{x}$, where $q^2(\bar{x})$ is the

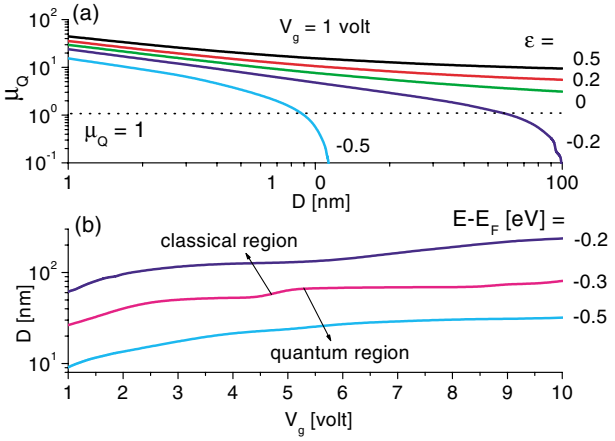

FIG. 3 (color online). (a) The normalized quantum CL law μ_Q as a function of gap spacing D (nm) for various values of $\epsilon = (E - E_F)/eV_g = 0.5$ to -0.5 at gap voltage $V_g = 1$ V. (b) The boundary of the transition from the quantum region (small D) to the classical region (large D) for $E - E_F$ [eV] = -0.2, -0.3, and -0.5.

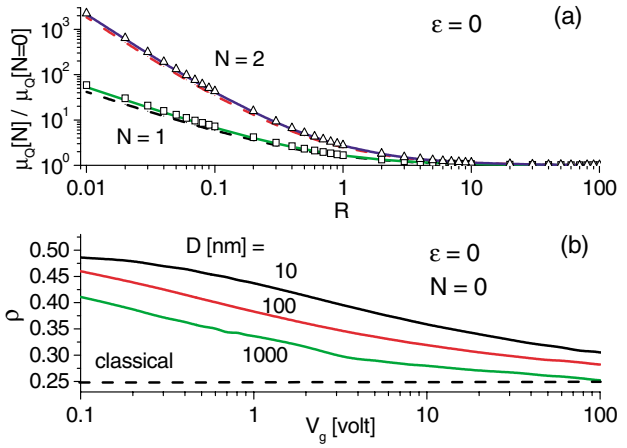

FIG. 4 (color online). (a) The ratio of $\mu_Q[N]$ to $\mu_Q[N=0]$ as a function of the normalized electrode's curvature R at gap voltage $V_g = 1$ V for gap spacing: $D = 10$ nm (solid line) and $D = 100$ nm (dashed line), where $N = 1$ and $N = 2$ are cylindrical and spherical geometry, respectively. The symbols are for $V_g = 10$ V and $D = 10$ nm: triangle ($N = 2$) and rectangle ($N = 1$). (b) The mean location of electrons ρ as a function of gap voltage V_g (volt) for various values of gap spacing $D = 10$, 100, and 1000 nm. The classical limit is $\rho = 0.25$ (dashed line).

normalized 1D electron density profile calculated from solving Eqs. (4) and (5) at $\mu = \mu_Q[1\mathrm{D}]$ at $N = 0$. Figure 4(b) gives the values of ρ as a function V_g at $D = 10$ nm, $D = 100$ nm, and $D = 1000$ nm. In the limit of $\lambda \gg 1$ and $\phi_g \gg 1$, we have $q^2 \propto \bar{x}^{-2/3}$, ρ becomes $\rho = 1/4$, and Eqs. (8) recover the classical limits [3].

To see the effects of the quantum corrections, consider a circular emitter of radius $R = 5$ nm subject to a gap voltage $V_g = 9$ V with a gap spacing $D = 100$ nm, with an average electric field of 0.09 V/nm. Our model yields a maximum current density of 7.7×10^6 A/cm^2, in which the quantum enhancement and 2D geometrical enhancement is, respectively, $\mu_Q = 1.65$ and 7.4 [cf. Eq. (8b)]. This current density happens to be in the range of 6 to 7×10^6 A/cm^2, a value that is inferred from an advanced multiwall carbon nanotube emitter with a radius of 5 nm, subject to a gap voltage of about 120 V across a separation of 1.34 μm [16]. Note that the average electric field in the latter case is also 0.09 V/nm, with no electrical breakdown reported [16].

In this formulation, we have assumed a slowly varying electron density in the gap, where the electron exchange-correlation potential depends only on the local electron density (using LDA). This assumption is valid since the spatial variation of electron density in our calculation is on the order of gap spacing which is larger than the atomic scale (not shown). Note this model has also ignored the electron emission mechanisms in the vicinity of the surface, where the surface properties of the materials such as local energy of states, dipole due to charge penetration, and nature of ion lattice are ignored. It is important to note that these effects may become important when the gap spacing is extremely small, such as $D < 1$ nm. The effects of electron density inhomogeneity, the comparison of other density functional theories, quantum fluctuations, and surface properties will be the subjects of future studies.

In conclusion, using mean field theory and LDA theory, a consistent and exact 1D quantum mechanical model of Child-Langmuir law, including the electron exclusion principle, is established for planar, cylindrical, and spherical geometries. For the first time, a new scaling of the Child-Langmuir law in the quantum regime, $J_Q \propto V_g^{1/2}$ and $J_Q \propto D^{-4}$, is established for small V_g and D. The model provides an upper limit of electron current density for steady-state electron beam propagation in a nanosized gap, and it is independent of the nature of the electron emission process. A simple 2D quantum model is also developed based on the exact 1D model.

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