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# Dielectric-environment mediated renormalization of many-body effects in a one-dimensional electron gas

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# Dielectric environment mediated renormalization of many-body effects in one dimensional electron gas

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Relaxing the assumption of an “infinite and homogenous background”, the dielectric response function of one-dimensional (1D) semiconducting nanowires embedded in a dielectric environment is calculated. It is shown that a high- $\kappa$  (higher than semiconductor dielectric constant) dielectric environment reduces the screening by the free carriers inside the nanostructure, whereas a low dielectric constant environment increases the Coulombic interaction between free carriers and enhances the strength of screening function. In the long wavelength limit, dielectric screening and collective excitations of electron gas are found to be strongly influenced by the environment. Behavior of static dielectric function is particularly addressed at a specific wavevector  $q = 2k_F$ ; a wavevector that ubiquitously appears in charge transport in nanostructures. It is shown that the exclusion of the dielectric mismatch effect in free carrier screening results in erroneous charged impurity scattering rate, particularly for nanowires embedded in low- $\kappa$  dielectrics.

Low-dimensional structures such as semiconducting nanowires (1D) are being investigated intensively for their potential applications in high-speed electronic and optical devices<sup>1</sup>. These nanowires can either be freestanding, or can be coated with different dielectric environments appropriate to device application. For example, in nanowire-based field effect transistors (FETs), they are usually coated with high- $\kappa$  dielectrics (HfO<sub>2</sub>, ZrO<sub>2</sub>, etc.)<sup>2</sup> for improved charge control and high electron mobility<sup>3</sup>. On the other hand, for exciton-based devices, use of low- $\kappa$  (lower than semiconductor dielectric constant  $\epsilon_s$ ) dielectric is beneficial as it enhances the excitonic binding energy<sup>5</sup>. These advantages in electronic and optical properties stem from the fact that the Coulomb interaction between carriers and/or impurities inside the nanowires can be altered by altering the environment. This tunability of the carrier-carrier interaction by dielectric environment is expected to modify many-body effects such as dielectric screening by one dimensional electron gas (1DEG) inside the nanowire.

Dielectric screening by free carriers plays a crucial role in the transport quantities (conductivity, mobility, etc) of a nanostructure. In a scattering event, the momentum-relaxation time ( $\tau$ ) strongly ( $\tau \sim |\epsilon(q, 0)|^{-2}$ ) depends on the free electron screening inside the semiconductor. Hence an accurate knowledge of dielectric screening is necessary for a precise prediction of transport coefficients of a nanowire. The dielectric function of a semiconductor nanowire is composed of i) ionic ( $\epsilon^{ion}$ ) and ii) electronic ( $\epsilon^{el}$ ) contributions.  $\epsilon^{ion}$  is an inherent property (crystal property) of semiconductors, while  $\epsilon^{el}$  (commonly known as the screening function) depends on the magnitude of the electron-electron interaction inside a material. As the dielectric environment can alter the Coulomb potential inside a nanowire, it is expected that dielectric environment will have a pronounced effect of the free electron screening<sup>6</sup>. Previous models<sup>7-10</sup> for the dielectric func-

tion of 1DEG assumes that the electron gas has a infinite homogenous background having dielectric constant ( $\epsilon_s$ ) same as the semiconductor. For a nanowire of few nm radius, “infinite background” approximation breaks down and at the nanowire/environment interface “homogenous background” assumption fails. In this work, assumptions are relaxed. By incorporating the dielectric mismatch factor at the nanowire/environment interface, a consistent theory of dielectric function is presented following the method of “self consistent field”<sup>4,8,11</sup> (also known as the random-phase approximation or RPA).

It is worthwhile to mention that the dielectric mismatch effect on the static screening is incorporated in recent numerical approaches (see Ref.<sup>4</sup>) for Si/SiO<sub>2</sub> nanowires. The main concern of the work by Jin *et. al* was to investigate the surface roughness and the diameter-dependent electron mobility in nanowires mostly restricted to Si/SiO<sub>2</sub> nanowires. The effect of the dielectric environment on the free carrier screening was not analyzed and hence the idea remained dormant so far. Here, following the general formalism developed in Ref.<sup>4</sup>, and including the dielectric mismatch effect, an analytical expression of dynamic dielectric function is evaluated. Both the static dielectric function and the collective excitations of 1DEGs in the long-wavelength limit are found to be solely determined by the dielectric environment. The importance of the modification of the static electronic screening by the dielectric environment is illustrated by calculating the screened ionized impurity scattering rates for nanowires embedded in both high and low- $\kappa$  dielectrics.

We consider an infinitely long semiconductor wire (dielectric constant  $\epsilon_s$ ) of a radius ( $R$ ) of few nanometers embedded in a dielectric (dielectric constant  $\epsilon_e$ ) environment. To investigate the dielectric response of the electron gas inside the wire, we place an oscillating test charge at  $(\mathbf{r}_0, z_0) = (0, 0)$  of density  $n_0(r, t) = e\delta(\mathbf{r})e^{-i\omega t}$ . This test charge creates an oscillating potential  $V_0(r, z)e^{-i\omega t}$  in the nanowire and in response to this

85 perturbation, free electrons inside the nanowire rearrange  
86 themselves to screen the field. The resultant Hamiltonian  
87 of electrons confined in the wire is  $H = H_0 + V(\mathbf{r}, t)$ ,  
88 where  $V(\mathbf{r}, t)$  is the self-consistent potential in response  
89 to the perturbation  $V_0(\mathbf{r}, t)$ . The unperturbed single-  
90 particle Hamiltonian  $H_0 = \mathbf{p}^2/2m^* + V_{con}(r)$  satisfies  
91 the Schroedinger equation  $H_0|n, k\rangle = \mathcal{E}_{n,k}|n, k\rangle$ . Here  
92  $m^*$  is the effective mass of electrons,  $k$  is the one di-  
93 mensional wave vector,  $|n, k\rangle$  and  $\mathcal{E}_{n,k}$  are the eigen-  
94 vectors and eigen-energy of the unperturbed Hamilto-  
95 nian, and  $V_{con}(r)$  is the confinement potential for elec-  
96 trons inside the nanowire. Assuming electrons are con-  
97 fined in a infinite-barrier potential, the eigen-energies  
98 are  $\mathcal{E}_{n,k} = \mathcal{E}_n + \hbar^2 k^2/2m^*$ , where  $\mathcal{E}_n$  is the ground  
99 state energy of the  $n$ th 1D subband and  $\hbar$  is the re-  
100 duced Planck constant. The corresponding wavefunc-  
101 tion is  $\Psi_{n,k}(r, z) = \langle r|n, k\rangle = \phi_n(r) \cdot [\exp(ikz)/\sqrt{L}]$ ,  
102 where  $\phi_n(r)$  is the radial part and  $L$  is the length of  
103 the nanowire. The dielectric function of an electron gas  
104 is defined by the relation<sup>12</sup>

$$V_{nn'} = \sum_{mm'} \epsilon_{nn', mm'}^{-1}(q, \omega) V_{mm'}^0, \quad (1)$$

105 where  $\epsilon_{nn', mm'}^{-1}(q, \omega)$  is the four dimensional dielectric  
106 matrix and  $V_{ij}(V_{ij}^0) = \langle j, k + q|V(V_0)|i, k\rangle$  are the tran-  
107 sition matrix element between states  $|i, k\rangle$  and  $|j, k + q\rangle$ .  
108 Diagonal elements of the dielectric matrix represent the  
109 intrasubband polarization of the 1DEG whereas, the off-  
110 diagonal terms result from inter-subband transitions. In  
111 the size quantum limit (SQL) carriers are confined in the  
112 lowest ground state and intersubband separation is large,  
113 and the dielectric function becomes a scalar quantity.

114 The self-consistent potential contains both the origi-  
115 nal perturbation as well as the screened potential by  
116 the mobile charges, i.e.  $V(\mathbf{r}, t) = V_0(\mathbf{r}, t) + V_{sc}(\mathbf{r}, t)$ .  
117 For the evaluation of the dielectric response of a 1D  
118 electron gas, it is imperative to calculate the screening  
119 potential  $V_{sc}$  (see eq. 1)). The self-consistent poten-  
120 tial  $V(\mathbf{r}, t)$ , upon acting on state  $|n, k\rangle$  mixes it with  
121 other states such that wave function becomes  $\Psi(r, t) =$   
122  $|n, k\rangle + \sum_{n', q} b_{k, k+q}(t)|n', k + q\rangle$ . The coefficient  $b_{k, k+q}(t)$   
123 is given by time dependent perturbation theory<sup>13</sup>

$$b_{k, k+q}(t) = \frac{V_{nn'}(q)e^{-i\omega t}}{\mathcal{E}_{n'}(k + q) - \mathcal{E}_n(k) - \hbar\omega}, \quad (2)$$

124 where,  $V_{nn'} = \langle n', k + q|V|n, k\rangle$  is the matrix el-  
125 ement between state  $|n, k\rangle$  and  $|n', k + q\rangle$ . The  
126 perturbation-induced charge density is  $n^{ind}(r, t, z) =$   
127  $-2e \sum_{k, nn'} f_n^0(k) [|\Psi(r, t)|^2 - |\Psi_{n,k}(r, z)|^2]$ , where,  $e$  is  
128 the charge of an electron and  $f_n^0(k)$  denotes the equilib-  
129 rium Fermi-Dirac occupation probability of a state  $|n, k\rangle$   
130 such that  $2 \sum_{n, k} f_n^0(k) = n_{1d}$ ,  $n_{1d}$  being the equilibrium  
131 homogeneous unperturbed electron gas density. Assum-  
132 ing that the perturbation is weak enough such that the

133 response is linear, and neglecting terms  $b_{n, k+q}^2$  and higher  
134 orders, the induced charge density can be written as  
135  $n^{ind}(r, t) = -e \sum_{nn'} \phi_n(r) \phi_{n'}(r) V_{nn'} \mathcal{F}_{nn'}(q, \omega) e^{iqz} e^{i\omega t} +$   
136  $c.c.$ , where  $c.c.$  denotes the *complex conjugate* and  
137  $\mathcal{F}_{nn'}(q, \omega)$  is the polarization function<sup>13</sup> (Lindhard func-  
138 tion) obtained by summing the Feynman diagram of  
139 electron-electron interaction containing single fermion  
140 loop<sup>7,14</sup>,

$$\mathcal{F}_{nn'}(q, \omega) = \frac{2}{L} \sum_k \frac{f_n^0(k) - f_{n'}^0(k + q)}{\mathcal{E}_{n'}(k + q) - \mathcal{E}_n(k) - \hbar\omega}. \quad (3)$$

141 Note that the induced charge density has the same har-  
142 monic dependence as the self consistent potential. The  
143 induced charge density is related to the screening po-  
144 tential by Poisson's equation  $\nabla^2 V_{sc}(\mathbf{r}) = en^{ind}(\mathbf{r})/\epsilon_0\epsilon_s$ ,  
145 where  $\epsilon_0$  is the free-space permittivity. Expressing  
146 screening potential in Fourier components  $V_{sc}(r, z) =$   
147  $\sum_{-\infty}^{\infty} v_{sc}(r, q) e^{iqz}$ , where  $q = k' - k$ , one obtains the  
148 differential equation for the screening potential

$$\frac{1}{r} \frac{d}{dr} \left( r \frac{dv_{sc}}{dr} \right) - q^2 v_{sc} = \begin{cases} en^{ind}(r)/\epsilon_0\epsilon_s, & r \leq R \\ 0, & r \geq R. \end{cases} \quad (4)$$

149 The Green's function appropriate to the above differen-  
150 tial equation with dielectric mismatch effect is<sup>3,4,15</sup>

$$G(r, r', q) = \frac{1}{\pi} \left[ \underbrace{I_0(q, r_{<}) K_0(q, r_{>})}_{g^{inhom}(r, r')} + \underbrace{\mathcal{U}(qR) I_0(qR) K_0(qR')}_{g^{hom}(r, r')} \right]$$

$$\mathcal{U}(x) = \frac{(\epsilon_s - \epsilon_e) K_0(x) K_1(x)}{\epsilon_e I_0(x) K_1(x) + \epsilon_s I_1(x) K_0(x)} \quad (5)$$

151 where,  $g^{hom(inhom)}(r, r')$  is the homogenous  
152 (inhomogenous) part of the Green's function,  
153  $r_{<(>)} = \min(\max)[r, r']$ , and  $I_n(\dots)$  and  $K_n(\dots)$  are  
154 the  $n$ th order modified Bessel functions. For large  $x$   
155 ( $x > |n^2 - 1|$ ),  $I_n(x) \approx e^x/\sqrt{2\pi x}$ ,  $K_n(x) \approx e^{-x}\sqrt{2\pi/x}$   
156 and the function  $\mathcal{U}(qR) \rightarrow (\pi\gamma/2)e^{-2qR}$ , where  
157  $\gamma = (\epsilon_s - \epsilon_e)/(\epsilon_s + \epsilon_e)$  is the dielectric mismatch factor.  
158 The tunability of the strength of the Green's function  
159 arises through its dependence on  $\gamma$ , which enhances  
160 (reduces) the strength for  $\epsilon_s > \epsilon_e$  ( $\epsilon_s < \epsilon_e$ ). For an  
161 infinite homogeneous environment ( $\epsilon_e = \epsilon_s$ ),  $\gamma = 0$ , and  
162 the Green's function is independent of the dielectric  
163 environment. Using the above Green's function, the  
164 induced potential inside the nanowire can be written  
165 as  $v_{sc}(r, q) = e/4\pi\epsilon_0\epsilon_s \int_0^R G(r, r', q) n^{ind}(r') r' dr'$ <sup>16</sup>. In  
166 the size quantum limit (SQL), the nanowire is thin,  
167 ( $R < \lambda_{dB}, \lambda_{dB}$  is de Broglie wavelength of an electron)  
168 and only the lowest subband is populated. Moreover, for  
169 a thin nanowire, inter-subband separation energy is large  
170 ( $\Delta\mathcal{E}_n \propto 1/R^2$ ) such that inter-subband transition can be  
171 neglected ( $n = n' = 1$ ). In such a scenario, the dielectric  
172 matrix becomes scalar, i.e.  $\epsilon_{nn'}(q, \omega) \rightarrow \epsilon_{11}(q, \omega)$ .  
173 Assuming  $\phi_{n=1}(r) \approx 1/\sqrt{\pi R^2}$ , the dynamic dielectric  
174 function of an 1DEG at temperature  $T = 0$  is<sup>17</sup>

$$\epsilon_{1d}(q, \omega, \mathcal{E}_F) = 1 - \frac{e}{4\pi\epsilon_0\epsilon_s V_{11}} \int_0^R \phi_1^2(r)r \int_0^R G(r, r') n^{ind}(r') r' dr' dr$$

$$= 1 + \frac{1}{\pi a_B^* R^2} \frac{F(x)}{q^3} \ln \left| \frac{(q + 2k_F)^2 - (\frac{2m^*\omega}{\hbar q})^2}{(q - 2k_F)^2 - (\frac{2m^*\omega}{\hbar q})^2} \right|, \quad (6)$$

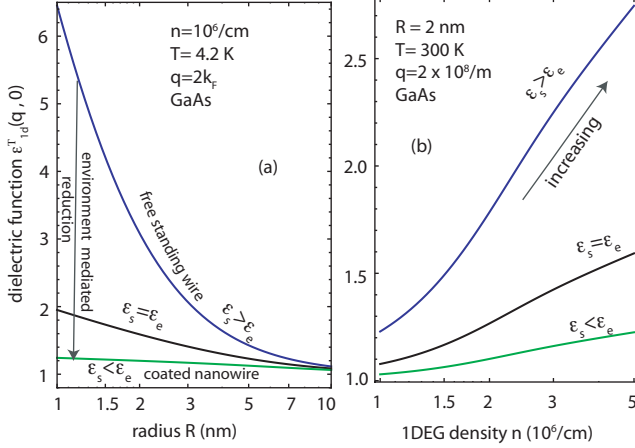


FIG. 1. Dielectric function of a nanowire a) with nanowire radius ( $R$ ) and b) as a function of carrier density ( $n$ ) for three different dielectric environments of  $\epsilon_e = 1$  (upper branch),  $\epsilon_e = \epsilon_s = 13$  (middle) and  $\epsilon_e = 100$  (lower branch).

where  $x = qR$  a dimensionless quantity,  $F(x) = \left[ \frac{1}{2} + I_1(x)[\mathcal{U}(x)I_1(x) - K_1(x)] \right]$ ,  $a_B^* = 4\pi\epsilon_0\epsilon_s\hbar^2/m^*e^2$  is the effective bulk Bohr radius,  $k_F = \pi n_{1d}/2$  is the Fermi wavevector and  $\mathcal{E}_F = \hbar^2 k_F^2 / (2m^*)$  is the corresponding Fermi energy. The logarithmic term in Eq.6 is results from the Lindhard function  $\mathcal{F}_{11}(q, \omega)$  which has been evaluated analytically in the SQL<sup>7</sup>. In the context of charge transport inside the nanowire, the static part of the dielectric function  $\epsilon_{1d}(q, \omega = 0)$  is relevant. In the long wavelength ( $q \ll 2k_F$ ) limit, the static dielectric function  $\epsilon_{1d}(q, 0)$  for a thin nanowire ( $qR \rightarrow 0$ ) becomes

$$\epsilon_{1d}(q, 0) = 1 - \frac{e^2}{2\pi\epsilon_0\epsilon_e} [\ln(qR)] \mathcal{D}_{1d}(\mathcal{E}_F), \quad (7)$$

where,  $\mathcal{D}_{1d}(\mathcal{E}_F) = (1/\pi\hbar)\sqrt{2m^*/\mathcal{E}_F}$  is the 1D density of states per unit length at Fermi energy  $\mathcal{E}_F$ . In sharp contrast to previous models<sup>12</sup>, the dielectric constant of the environment ( $\epsilon_e$ ) instead of the semiconductor itself ( $\epsilon_s$ ), determines the long-wavelength behavior of the static dielectric function.

For large momentum ( $q \gg 2k_F$ ),  $\epsilon_{1d}(q, 0) \rightarrow 1$  as the second term of Eq. 6 falls off rapidly ( $q^{-5}$ ) with  $q$ . For a degenerate 1DEG in SQL, only backscattering is allowed, which leads to a momentum transfer  $q = 2k_F$  in any intrasubband elastic scattering process. As a result,  $\epsilon_{1d}(q = 2k_F, 0)$  plays an important role in momentum relaxation rate calculation. In the static limit ( $\omega = 0$ ),

the dielectric function  $\epsilon_{1d}(q, 0)$  at  $T = 0$  is singular for  $q = 2k_F$ . This divergence is related to Peierl's instability, which is a characteristic signature of a 1DEG. At finite temperature, smearing of the Fermi function removes this singularity. The static dielectric function at  $T \neq 0$  is given by Maldague's prescription<sup>19</sup>

$$\epsilon_{1d}^T(q, 0) = \int_0^\infty d\mathcal{E} \epsilon_{1d}(q, 0, \mathcal{E}) \left[ 4k_B T \cosh^2 \left[ \frac{\mathcal{E} - \mathcal{E}_F}{2k_B T} \right] \right]^{-1}. \quad (8)$$

Fig.1a) shows the static dielectric function of a GaAs nanowire at  $q = 2k_F$  with nanowire radius  $R$  for three different dielectric media. Note that even negligible smearing of Fermi distribution at  $T = 4.2$  K is enough to remove the divergence at  $q = 2k_F$ . For coated nanowires with  $\epsilon_e > \epsilon_s$ , dielectric screening is strongly reduced as shown in Fig. 2 b). At large radius ( $R \gg 1/4k_F$ ), the nanowire tends to the bulk structure and the dielectric mismatch effect on the screening function vanishes. With increasing carrier density, dielectric screening inside the nanowire increases (see Fig. 1b) maintaining the effect of dielectric environment intact. At higher carrier densities, more than one subband is populated and inter-subband contribution to the total dielectric function should be taken into account for a complete description of free electron screening inside the nanowire. With increasing temperature, thermal fluctuation reduces the free electron screening inside the nanowire and the effect of environmental dielectric on the screening function is partially washed away (see Fig. 2a).

As the dynamic ( $\omega \neq 0$ ) dielectric function  $\epsilon_{1d}(q, \omega)$

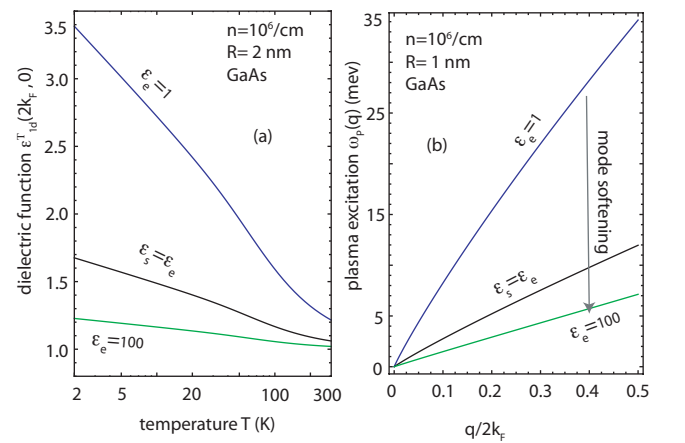


FIG. 2. a) Dielectric function of a nanowire with temperature ( $T$ ) and b) plasma frequency of an 1DEG with wavevector ( $q$ ) for three different dielectric environments.

contains the dielectric mismatch factor, collective excitations of the 1DEG is also expected to depend on the dielectric environment. Collective excitation of an electron gas is defined as the pole of the full dynamic dielectric function, i.e. by  $\epsilon_{1d}(q, \omega_p) = 0$ , where  $\omega_p$  is the plasma frequency of the electron gas. Fig.2b) shows the plasma dispersion of intra-subband collective excitation of a thin nanowire ( $R = 2\text{nm}$ ) for different dielectric environments. For  $q < 1/2R$ , the dielectric environment has a finite effect on the collective excitation frequency of 1DEG. The softening of plasma frequency with high- $\epsilon_e$  dielectric environment is the consequence of the reduction of Coulomb interaction between electrons and the positive background, which acts as a restoration force of the collective oscillation of the electron gas. For small  $q$ , the frequency of collective excitations goes to zero for all dielectric environment following the relation  $\omega_p(q) \approx \omega_0 q \sqrt{-\ln(qR)}$ , where  $\omega_0 = \sqrt{n_{1d}e^2/(4\pi\epsilon_0\epsilon_e m^*)}$ . Note the explicit appearance of  $\epsilon_e$  in  $\omega_0$  highlights the role of environment in collective excitation of 1DEG inside the wire.

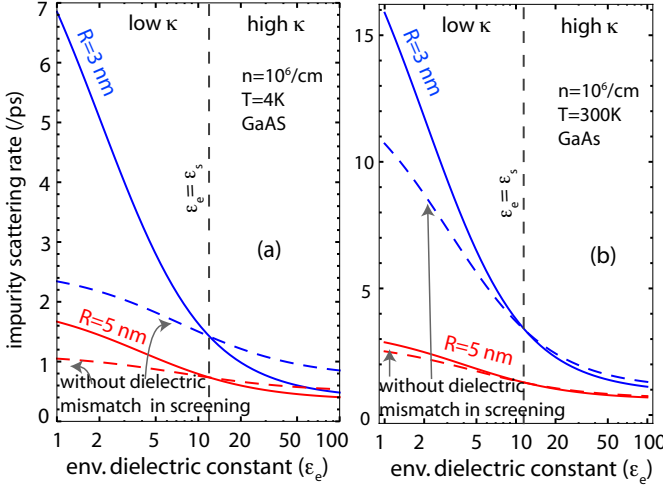


FIG. 3. Screened Coulomb scattering rate with (solid) and without (dashed) incorporating the dielectric mismatch in static screening at a) low temperature, and at b) room temperature as a function of dielectric constant of the environment. Here we assumed an impurity density  $n_{imp} = 2.5 \times 10^5/\text{cm}$

A typical example where the static dielectric function plays a crucial role is the determination of charged impurity scattering rate in semiconductor nanostructures. Fig.3(a) shows the screened Coulomb scattering rates at low temperature with (solid lines) and without (dashed lines) accounting the dielectric mismatch effect in free carrier screening for an impurity point charge  $e$  located on the axis of the nanowire. Here, we use the Coulomb potential derived in Ref.<sup>3</sup>. Note that the exclusion of the dielectric mismatch effect in the screening underestimates (overestimates) the scattering rate (see Fig.3(a)) for low- $\kappa$  (high- $\kappa$ ) dielectric medium surrounding thin ( $R \leq 5$

nm) nanowires. At room temperature, weak free carrier screening results in higher scattering rate (see Fig.3(b) compared to Fig.3(a)). At room temperature, the dielectric mismatch effect on the free carrier screening can be neglected for high- $\kappa$  dielectric environments, although for low- $\kappa$  environments, inclusion of the dielectric mismatch effect in screening is necessary for an accurate evaluation (see Fig.3(b)) of scattering rates.

The length scale at which dielectric environment plays an important role can be determined by investigating the behavior of  $\mathcal{U}(qR)$ . For large  $qR$ ,  $\mathcal{U}(qR) \sim e^{-4k_F R}$ . Hence for  $R \gg 1/(4k_F)$ ,  $\mathcal{U}(qR)$  becomes negligible and the dielectric effect vanishes. For numerical estimates, at carrier density  $n_{1d} = 10^6/\text{cm}$  dielectric effect vanishes for  $R \gg 2\text{ nm}$ , whereas at lower density ( $n_{1d} = 10^5/\text{cm}$ ) environmental effect on quantum screening function persists for wire radius up to  $R \approx 20\text{ nm}$ .

We have assumed an infinite confining potential for electron inside the wire. Relaxing this assumption will result in electron mass enhancement due to leaking of wavefunction into the barrier. For high- $\kappa$  oxides the typical barrier height is  $\sim 1\text{ eV}$ , for which nominal increase in electron mass can be neglected<sup>18</sup>. The assumption of constant radial part of the wavefunction is justified for thin nanowires. Choosing a different form for the radial part will change the absolute value of screening function for thick (for large  $R$  dielectric environment effect reduces anyway) wires keeping the relative effect of environments unchanged.

In conclusion, we have shown that the free electron screening inside a nanowire depends on the environment surrounding it. For a nanowire coated with a high- $\kappa$  dielectric, Coulomb perturbation inside the nanowire is poorly screened compared to a freestanding nanowire. It is shown that both the static dielectric function, and the plasma dispersion in the long-wavelength limit gets modified by the environment. The length-scale at which the environment has substantial effect on the electron gas inside the nanowire was identified. The results are analytical and will be useful for accurate prediction of transport coefficients in nanowire-based electronic devices.

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<sup>6</sup> One such example is dielectric environment mediated free electron screening in graphene, where an average dielectric constant of graphene  $\epsilon_{gr}^{avg} = (\epsilon_e^t + \epsilon_e^b)/2$  is used in the Thomas-Fermi screening function. Here  $\epsilon_e^t(\epsilon_e^b)$  is the dielectric constant of top (bottom) environment of graphene and the crystal property of atomically thin (monolayer 0.3 nm) graphene is neglected. For a nanowire of radius few nm, crystal property of the semiconductor can not be neglected and a rigorous model containing both  $\epsilon_e$  and  $\epsilon_s$  is necessary.
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