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Dimensionality Effects on Trap-Assisted Recombination: The Sommerfeld Parameter

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Abstract. In the context of condensed matter physics, the Sommerfeld parameter describes the enhancement or suppression of free-carrier charge density in the vicinity of a charged center. The Sommerfeld parameter is known for three-dimensional systems and is integral to the description of trap-assisted recombination in solids. Here we derive the Sommerfeld parameter in one and two dimensions and compare with the results in three dimensions. We provide an approximate analytical expression for the Sommerfeld parameter in two dimensions. Our results indicate that the effect of the Sommerfeld parameter is to suppress trap-assisted recombination in decreased dimensionality.

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‡ Deceased.

1. Introduction

Charged defects and impurities play an important role in condensed matter systems, leading to a variety of physics including as centers of carrier recombination. In the presence of a charged center, the free-carrier wavefunction is perturbed, leading to an enhancement or suppression of the carrier charge density in the vicinity of the center. This perturbation has been thoroughly analyzed in the case of bulk material and is commonly quantified as the Sommerfeld parameter [1, 2, 3, 4, 5]. The Sommerfeld parameter also arises in fields other than condensed matter physics, for example, in the description of dark matter in high-energy astrophysics [6, 7, 8].

Understanding trap-assisted recombination at defects or impurities is of utmost importance for improving device performance. In optoelectronic devices such as light-emitting diodes or solar cells, the so-called Shockley-Read-Hall process allows carriers to recombine nonradiatively, transferring the excitation energy into lattice vibrations and reducing the emission efficiency. Point defects and impurities may also act as charge traps, capturing free carriers and degrading performance. First-principles formulations to evaluate nonradiative recombination rates exist [9, 10, 11, 12], and the calculated rates are scaled by the Sommerfeld parameter when a charged center is involved. For example, the nonradiative capture coefficent is given by $C = s(T)\tilde{C}$, where $s(T)$ is the temperature-dependent Sommerfeld parameter and $\tilde{C}$ is the capture coefficient calculated in a neutral defect-containing supercell. This scaling is necessary because typical supercells used in first-principles calculations are insufficiently large to describe the long-ranged Coulomb potential of the charged center. The Sommerfeld parameter also plays a role in radiative capture [13] and trap-assisted Auger-Meitner recombination [14].

Many relevant device architectures involve lower-dimensional structures. For example, light-emitting diodes utilize quantum wells, in which carriers are confined and behave as if they are quasi-two-dimensional. Going further, semiconductor nanowires, in which confinement of carriers leads to quasi-one-dimensional behavior, are being explored for next-generation optoelectronic devices [15]. Semiconductor nanowires [16] and gate-defined quasi-one-dimensional wires derived from a two-dimensional electron gas [17] have been employed in the search for Majorana bound states. Devices are getting ever smaller, and quantum effects and dimensionality play a larger role. In addition, two-dimensional materials, such as hexagonal boron nitride, are being considered for electronic devices through the construction of van der Waals heterostructures [18]. Two-dimensional materials are also promising hosts for quantum defects [19, 20, 21], particularly for applications in quantum metrology [22]. Quasi-one-dimensional materials, such as carbon nanotubes, are also being explored as hosts for quantum defects [23, 24]. Of course, lower-dimensional systems still exist in three dimensions; while the wavefunction in the confined directions is not constant, studying an idealized lower-dimensional system provides important insight into the effects of dimensionality since it allows focusing on the key long-range effects.

In this work, we assess the effect of dimensionality on trap-assisted recombination by studying the Sommerfeld parameter. We first review the derivation of the Sommerfeld parameter in three dimensions (3D) and then derive the Sommerfeld parameter in two (2D) and one (1D) dimensions, comparing to the case of 3D. We provide an approximate analytical expression for the temperature dependence in 2D and assess the accuracy of the utilized approximations in 2D and 3D. In 1D, an explicit formula cannot be obtained and instead direct numerical evaluation is used.

Overall we find that reduced dimensionality suppresses trap-assisted recombination through the Sommerfeld parameter. This result has important implications for device performance. We have implemented these developments in the latest version of the Nonrad code [25, 12], which is an open-source Python code that evaluates the nonradiative capture rate from first principles.

In Sec. 2, we formulate the problem of a charged center in an effective medium through the Wannier equation and derive the Sommerfeld parameter in different dimensions. We review the derivation of the Sommerfeld parameter in 3D in Sec. 2.1, and derive the Sommerfeld parameter in 2D in Sec. 2.2 and in 1D in Sec. 2.3. In Sec. 3, we discuss the results from our derivations, in particular assessing the effects of dimensionality and the numerical stability of the employed approximations. We comment on the implications of these results for devices and experiments in Sec. 4: Reduced recombination in lower dimensions will be favorable for device performance. Section 5 concludes the paper.

2. Derivation of the Sommerfeld Parameter

We seek to describe the perturbation of a carrier wavefunction in the presence of a Coulomb center. We will first focus on electrons and comment on the case of holes at the end of this section. We write down a single-particle Schrödinger equation for an electron in a periodic potential in the presence of a perturbation (in SI units),

$$\left[-\frac{\hbar^2}{2m_e}\nabla^2 + V(\mathbf{r}) + U(\mathbf{r})\right]\psi = E\psi \,, \tag{1}$$

where m_e is the free electron mass and $V(\mathbf{r})$ is the periodic potential that the electron experiences. U is the Coulomb center potential and is given by $U(\mathbf{r}) = (Z/4\pi\epsilon_r\epsilon_0)(e^2/|\mathbf{r}|)$. Z is the charge of the Coulomb center (in units of the elementary charge e), ϵ_0 is the vacuum permittivity, and ϵ_r is the static relative permittivity of the material.

The Coulomb center potential U constitutes a minor and slowly varying perturbation, and therefore the Bloch functions form a natural basis for expanding the eigenfunction ψ. Luttinger and Kohn [26] provided an ansatz for the wavefunction, thus providing the foundation of effective mass theory,

$$\psi(\mathbf{r}) = \sqrt{\mathcal{N}_0\Omega_0}\,\phi(\mathbf{r})\,u_{\mathbf{k_0}}(\mathbf{r}) \,, \tag{2}$$

where $u_{\mathbf{k_0}}$ is the unperturbed Bloch function of the crystal at the band extremum located at wavevector $\mathbf{k}_0$. $\mathcal{N}_0$ is the number of unit cells that the wavefunction extends over. Ω_0 is the volume of the unit cell in 3D; in 2D it is the area, and in 1D, the length of the unit cell. $\phi(\mathbf{r})$ is the envelope function, which we will solve for.

For an electron in an isotropic parabolic band, the energy $E \approx E_0 + \hbar^2|\mathbf{k}-\mathbf{k}_0|^2/2m^*$, where m^* is the band effective mass. Furthermore, we will assume that the band extremum occurs at the Γ point ($\mathbf{k}_0 = \mathbf{0}$) and that the extremum is non-degenerate. These assumptions do not affect the generality of our results, and we comment on their influence in Sec. 3. Under these assumptions, equation 1 may be reduced to the Wannier equation [27, 28, 29, 30, 2]

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2 + U(\mathbf{r})\right]\phi(\mathbf{r}) = \varepsilon\phi(\mathbf{r}) \,, \tag{3}$$

which may be solved for the envelope function ϕ. ε is the corresponding eigenenergy for the envelope function and is referenced to the band extremum E_0.

In deriving the Sommerfeld parameter, we are most interested in the continuum solutions of equation 3, i.e. $\varepsilon = \hbar^2 k^2/2m^* > 0$. Therefore k will be a good quantum number for the envelope function. The envelope function also implicitly depends on Z, which sets the Coulomb center potential. In the following sections, we will explicitly include the labels Z and k in the notation for the envelope function, $\phi_k^Z(\mathbf{r})$. An important limit to consider is the absence of the Coulomb center potential, where $Z = 0$. In this case, it must be true that

$$\phi_k^0(r) = e^{ikr}/\sqrt{\mathcal{N}_0\Omega_0}\ , \tag{4}$$

or in other words, the wavefunction in equation 2 should be equivalent to the unperturbed Bloch function of the crystal $u_{\mathbf{k}_0}$.

The above arguments can be generalized to the case when the carrier corresponds to a hole in the valence band by a judicious change of sign. What matters in the end is whether the Coulomb potential corresponds to an attractive or repulsive potential. In other words, one should regard Z not as the Coulomb center charge, but as the product of the Coulomb center charge and the charge of the carrier (both in units of the elementary charge e). With this definition, $Z > 0$ ($Z < 0$) corresponds to a repulsive (attractive) potential.

2.1. Three Dimensions

First we review the derivation in 3D, as it will provide guidance for the derivation in 2D and 1D. In 3D, equation 3 is most readily solved in spherical coordinates. Standard separation of variables permits us to write

$$\phi_k^Z(\mathbf{r}) = R_{kl}(r)Y_{lm}(\theta,\varphi)\ , \tag{5}$$

where $R_{kl}(r)$ is a function of the radial variable r. $Y_{lm}(\theta,\varphi)$ are the spherical harmonics in the angular variables (θ,φ) and are indexed by l and m. Inserting equation 5 into equation 3 provides an equation to solve for the radial function,

$$\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\gamma}{r} + k^2 - \frac{l(l+1)}{r^2}\right) R_{kl}(r) = 0 \tag{6}$$

where $\gamma = 2Z/a^*$ and $a^* = 4\pi\epsilon_r\epsilon_0\hbar^2/(m^*e^2)$ is the effective Bohr radius.

The solutions to equation 6 have the form [5, 31, 32, 33]

$$R_{kl}(r) = C_{kl}\, e^{-ikr} r^l F(1+l-i\nu,\, 2l+2,\, 2ikr)\ , \tag{7}$$

where $\nu = \gamma/2k = Z/a^*k$ and C_{kl} is a normalization coefficient to be determined. F is the regular confluent hypergeometric series given by

$$F(\alpha,\beta,\xi) = 1 + \frac{\alpha}{\beta}\frac{\xi}{1!} + \frac{\alpha(\alpha+1)}{\beta(\beta+1)}\frac{\xi^2}{2!} + \dots\ . \tag{8}$$

At large distances ($r \to \infty$), equation 7 becomes

$$R_{kl}(r) = \frac{C_{kl}}{kr}\frac{\Gamma(2l+2)}{(2k)^l}\frac{e^{\pi\nu/2}}{|\Gamma(1+l+i\nu)|} \times \cos\left(kr - \nu\log(2kr) - \frac{\pi}{2}(l+1) - \sigma_l\right)\ , \tag{9}$$

where Γ is the Gamma function, and σ_l is the complex phase of the Gamma function, given by

$$\sigma_l = \arg\Gamma(1+l+i\nu)\ . \tag{10}$$

The wavefunctions of the continuous spectrum resemble spherical waves far from the Coulomb center.

To determine the normalization coefficient C_{kl}, we apply the normalization condition "in k scale" [31]:

$$\int_0^\infty dr\, r^2 R_{kl}(r) \int_{k-\Delta k}^{k+\Delta k} dk' R_{k'l}(r) = 1 \,, \tag{11}$$

where Δk is a small interval. Applying the normalization condition to the asymptotic form of the radial function (equation 9) we obtain

$$C_{kl} = \sqrt{\frac{2}{\pi}} \frac{k(2k)^l}{\Gamma(2l+2)} \sqrt{\frac{2\pi\nu}{e^{2\pi\nu}-1} \prod_{s=1}^{l} [s^2+\nu^2]} \,. \tag{12}$$

The spherical harmonics were convenient to solve equation 3. However, to satisfy equation 4 and derive the Sommerfeld parameter, it is more convenient to switch our approach to that of a scattering problem. For this, we utilize the partial-wave expansion [5],

$$\phi_k^Z(\mathbf{r}) = \frac{(2\pi)^{3/2}}{\sqrt{\mathcal{N}_0\Omega_0}} \frac{1}{4\pi k} \times \sum_{l=0}^{\infty} i^l (2l+1) e^{i\delta_l} P_l(\mathbf{k}\cdot\mathbf{r}/kr) R_{kl}(r) \,, \tag{13}$$

where δ_l are the scattering phases and P_l are the Legendre polynomials. R_{kl} is the radial wavefunction given in equation 7 with the normalization determined in equation 12. However, we have adjusted the normalization of equation 13 to be normalized over the volume of the crystal rather than all space, thus ensuring equation 4 is satisfied.

The Sommerfeld parameter $s(k)$ describes the enhancement or suppression of charge density in the vicinity of a charge center. Thus $s(k)$ is given by the ratio of the charge density in the presence of the Coulomb center ($Z \neq 0$) to the value in its absence ($Z = 0$). We write

$$s(k) = \frac{\left|\phi_k^Z(0)\right|^2}{\left|\phi_k^0(0)\right|^2} = \mathcal{N}_0\Omega_0 \left|\phi_k^Z(0)\right|^2 \,. \tag{14}$$

Note that the division by $\left|\phi_k^0(0)\right|^2$ implies that the choices of normalization conditions applied in equations 11, 12, and 13 ultimately do not matter, as long as they are applied consistently. Using equation 13, we obtain the result [2, 3]

$$s^{\mathrm{3D}}(k) = \frac{2\pi Z}{a^* k} \frac{1}{e^{2\pi Z/a^* k} - 1} \,, \tag{15}$$

where we have used the fact that $R_{kl}(0)$ is non-zero only for $l = 0$ and $F(\alpha, \beta, 0) = 1$, and we have restored the definition of ν.

For the purposes of trap-assisted recombination, information about the temperature dependence of the Sommerfeld parameter is particularly relevant. At a given temperature, there is a distribution of momenta present in the carriers of the system, which must be averaged over. The temperature-dependent Sommerfeld parameter in 3D, $s^{\mathrm{3D}}(T)$, is given by

$$s^{\mathrm{3D}}(T) = \frac{\int_0^\infty dk\, k^2\, s(k)\, e^{-\hbar^2 k^2/2m^* k_B T}}{\int_0^\infty dk\, k^2\, e^{-\hbar^2 k^2/2m^* k_B T}} \,. \tag{16}$$

As will be discussed in Sec. 3, equation 16 may be integrated numerically to obtain $s^{3D}(T)$ accurately [12]. Alternatively, if we assume that $k \ll 2\pi|Z|/a^*$, $s^{3D}(k)$ may be approximated as

$$s^{3D}(k) \approx \frac{2\pi|Z|}{a^* k} \begin{cases} 1 & Z < 0 \\ e^{-2\pi|Z|/a^* k} & Z > 0 \end{cases} . \tag{17}$$

For the attractive interaction, the integration in equation 16 can then be performed explicitly using equation 17. However, for the repulsive case we must also employ Laplace's method [34] to approximately evaluate the integral, introducing a second potential source of error. We can then arrive at an explicit formula for the temperature-dependent Sommerfeld parameter,

$$s^{3D}(T) = \begin{cases} \frac{4}{\sqrt{\pi}} \left[\frac{Z^2\theta_b}{T}\right]^{1/2} & Z < 0 \\ \frac{8}{\sqrt{3}} \left[\frac{Z^2\theta_b}{T}\right]^{2/3} \exp\left(-3\left[\frac{Z^2\theta_b}{T}\right]^{1/3}\right) & Z > 0 \end{cases} , \tag{18}$$

where $\theta_b = m^* e^4/[32 k_B (\epsilon_r \epsilon_0)^2 \hbar^2]$ is a parameter with units of temperature. (Equation 18 coincides with equation 4.5 of [2].)

The range of momenta over which we need to integrate, and hence the validity of the assumption $k \ll 2\pi|Z|/a^*$, depends on temperature. It is often assumed that $k \ll 2\pi|Z|/a^*$, and hence equation 18, is valid for all temperatures that are relevant in the context of recombination, but in Sec. 3 we will explicitly discuss the potential errors arising from the approximation.

2.2. Two Dimensions

In 2D, equation 3 is most readily solved in polar coordinates. Once again, separation of variables permits us to write the envelope function as

$$\phi_k^Z(\mathbf{r}) = R_{km}(r)\Theta_m(\theta) , \tag{19}$$

where

$$\Theta_m(\theta) = \frac{1}{\sqrt{2\pi}} e^{im\theta} . \tag{20}$$

The radial function R_{km} satisfies the equation

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{\gamma}{r} + k^2 - \frac{m^2}{r^2}\right) R_{km}(r) = 0 . \tag{21}$$

The solutions to equation 21 take a form similar to equation 7 [35, 36],

$$R_{km}(r) = C_{km} e^{-ikr} r^{|m|} F(|m| + \frac{1}{2} - i\nu, 2|m| + 1, 2ikr) . \tag{22}$$

At large distances $r \to \infty$, the radial equation in 2D takes on the asymptotic form

$$R_{km}(r) = \frac{2C_{km}}{\sqrt{2kr}} \frac{\Gamma(2|m|+1)}{(2k)^{|m|}} \frac{e^{\pi\nu/2}}{|\Gamma(|m| + \frac{1}{2} + i\nu)|} \times \cos\left(kr - \nu\log(2kr) - \frac{\pi}{2}(|m| + \frac{1}{2}) - \sigma_m\right) , \tag{23}$$

where

$$\sigma_m = \arg\Gamma(|m| + \frac{1}{2} + i\nu) \ , \tag{24}$$

is the complex phase of the Gamma function.

In 2D, the normalization condition in k scale is modified to be

$$\int_0^\infty dr\, r R_{km}(r) \int_{k-\Delta k}^{k+\Delta k} dk' R_{k'm}(r) = 1 \ , \tag{25}$$

where Δk is a small interval. We thus obtain that

$$C_{km} = \sqrt{\frac{k}{\pi}} \frac{(2k)^{|m|}}{\Gamma(2|m|+1)} \sqrt{\frac{2\pi}{1+e^{2\pi\nu}} \prod_{s=0}^{|m|-1} [(s+\frac{1}{2})^2 + \nu^2]} \ . \tag{26}$$

In 2D, the partial-wave basis (chosen to satisfy equation 4) is given by

$$\phi_k^Z(\mathbf{r}) = \frac{1}{\sqrt{\mathcal{N}_0 \Omega_0}} \frac{1}{\sqrt{k}} \times \sum_{m=0}^{\infty} i^m (2m+1) e^{i\delta_m} P_m(\mathbf{k}\cdot\mathbf{r}/kr) R_{km}(r) \ . \tag{27}$$

R_{km} is the radial wavefunction given in equation 22 with the normalization determined in equation 26. Applying equation 14 with the partial-wave expansion in equation 27 gives us the Sommerfeld parameter in 2D,

$$s^{\mathrm{2D}}(k) = \frac{2}{1+e^{2\pi Z/a^* k}} \ , \tag{28}$$

This result is remarkably similar to that in 3D (equation 15). Temperature averaging in 2D is performed with

$$s^{\mathrm{2D}}(T) = \frac{\int_0^\infty dk\, k\, s(k)\, e^{-\hbar^2 k^2/2m^* k_B T}}{\int_0^\infty dk\, k\, e^{-\hbar^2 k^2/2m^* k_B T}} \ . \tag{29}$$

Under the assumption that $k \ll 2\pi|Z|/a^*$, equation 28 may be approximated as

$$s^{\mathrm{2D}}(k) \approx 2 \begin{cases} 1 & Z < 0 \\ e^{-2\pi|Z|/a^* k} & Z > 0 \end{cases} \ . \tag{30}$$

For the attractive interaction, we immediately obtain the result that the Sommerfeld parameter is (approximately) independent of temperature. Again we apply Laplace's method for the repulsive case. We obtain the explicit formula for the temperature-dependent Sommerfeld parameter in 2D:

$$s^{\mathrm{2D}}(T) = \begin{cases} 2 & Z < 0 \\ \sqrt{\frac{8\pi}{3}} \left[\frac{8Z^2\theta_b}{T}\right]^{1/6} \exp\left(-3\left[\frac{Z^2\theta_b}{T}\right]^{1/3}\right) & Z > 0 \end{cases} \ , \tag{31}$$

where $\theta_b = m^* e^4/[32 k_B (\epsilon_r \epsilon_0)^2 \hbar^2]$ is a parameter with units of temperature.

2.3. One Dimension

The Coulomb potential in 1D has long been a subject of research interest—and controversy [37, 38, 39, 40, 41]. With respect to the definition of the Sommerfeld parameter, various arguments have shown that the bare Coulomb potential in 1D is impenetrable [42, 43, 44, 45, 46]. In other words, the wavefunction must be identically zero at the origin, due to the harsh divergence of the potential. We thus conclude that the Sommerfeld parameter is identically zero even for an attractive potential in 1D.

In some works a modified potential was utilized to soften the divergence [38, 39, 40, 47]; this approach allows us to gain insight into the physical behavior in 1D. The modification of the bare Coulomb potential is a pragmatic choice since most "one-dimensional" systems, e.g., nanotubes, are not strictly 1D. While there are several possible choices for the modified potential, the qualitative conclusions are unaffected by this choice. Here we will follow the approach of [47].

In 1D, there is only one coordinate to account for and no separation of variables is necessary to solve equation 3. As such, equation 3 is written as

$$\left(\frac{d^2}{dx^2} - \frac{\gamma}{|x| + x_0} + k^2\right)\phi_k^Z(x) = 0\ , \tag{32}$$

where x is the coordinate of interest and $-\infty < x < \infty$ (unlike the radial variable $0 \leq r < \infty$). x_0 provides a cusp-type cutoff to the Coulomb potential and softens the divergence. When $x_0 \to 0$, the bare Coulomb potential is obtained.

Equation 32 can be written in the form of the Whittaker equation [48, 32, 33] by a suitable change of variables $z = 2ik(|x|+x_0)$. We introduce ν', defined as $\nu' = |Z|/a^*k$, and first focus on the attractive case ($Z < 0$). With this transformation, we obtain

$$\left(\frac{d^2}{dz^2} + \frac{i\nu'}{z} - \frac{1}{4}\right)\phi_k^Z(x) = 0\ , \tag{33}$$

which is the special case of the Whittaker equation where $\mu = 1/2$ in equation 9.220.1 of [32]. For the repulsive case, we take $\nu' \to -\nu'$; we are then free to take $z \to -z$, leaving equation 33 unchanged. We thus find that the repulsive and attractive Sommerfeld parameter in 1D are identical.

Equation 33 has four possible solutions $W_{\pm i\nu}(\pm z)$, which are linear combinations of the regular and irregular confluent hypergeometric series. The regular confluent hypergeometric series (equation 8) was used in the derivation for both 2D and 3D; in 1D, the irregular series is also a valid solution. The explicit form of $W_{\pm i\nu}(\pm z)$ is given by equation 9.220.4 in [32].

The physically relevant solution to equation 33 is given by

$$\phi_k^Z(x) = AW_{-i\nu}(z) + BW_{i\nu}(-z)\ , \tag{34}$$

where A and B are normalization coefficients to be determined. Based on the physics, we know that the solution, which is non-zero at the origin for finite x_0, should be an even function and obey

$$\frac{d}{dz}\phi_k^Z(x)|_{x=0} = 0\ . \tag{35}$$

Introducing $D_0 = \frac{d}{dz}W_{-i\nu}(z)|_{x=0}$ and $D_1 = \frac{d}{dz}W_{i\nu}(-z)|_{x=0}$, we can apply equation 35 to write the envelope function (equation 34) as

$$\phi_k^Z(x) = N\left[D_1W_{-i\nu}(z) - D_0W_{i\nu}(-z)\right]\ , \tag{36}$$

where $N = A/D_1$ is a normalization coefficient to be determined.

The asymptotic form of $W_{i\nu}(z)$ as $z \to \infty$ is

$$W_{i\nu}(z) \sim e^{-z/2} z^{i\nu} \, . \tag{37}$$

In 1D, we apply the normalization condition

$$\int_{-\infty}^{\infty} dx \phi_k^Z(x) \int_{k-\Delta k}^{k+\Delta k} dk' \phi_{k'}^Z(x) = \frac{\pi}{\mathcal{N}_0 \Omega_0} \, . \tag{38}$$

(The chosen normalization condition enforces equation 4 and differs from normalization in higher dimensions since the partial-wave basis is not invoked.) We obtain

$$N = \sqrt{\frac{e^{-\pi\nu}}{2\mathcal{N}_0\Omega_0}} \left(|D_0|^2 + |D_1|^2 \right)^{-1/2} \, . \tag{39}$$

Applying equation 14 gives us the Sommerfeld parameter in 1D

$$s^{1\mathrm{D}}(k) = \frac{e^{-\pi\nu}}{2} \frac{|D_1 W_{-i\nu}(z_0) - D_0 W_{i\nu}(-z_0)|^2}{|D_0|^2 + |D_1|^2} \, , \tag{40}$$

where $z_0 = 2ikx_0$. Given the complexity of this expression, we do not attempt to obtain an analytical form for the temperature dependence of the Sommerfeld parameter in 1D. The temperature-dependent Sommerfeld parameter in 1D can be obtained by numerically integrating

$$s^{1\mathrm{D}}(T) = \frac{\int_0^\infty dk \, s(k) \, e^{-\hbar^2 k^2 / 2m^* k_B T}}{\int_0^\infty dk \, e^{-\hbar^2 k^2 / 2m^* k_B T}} \, . \tag{41}$$

3. Discussion

The Sommerfeld parameter as a function of momentum is shown in figure 1. Focusing first on the repulsive Sommerfeld parameter [figure 1(a)], we find that independent of dimensionality the Sommerfeld parameter is less than one, which leads to a suppression of trap-assisted recombination. In all cases, $s(k \to \infty) = 1$ as expected. We find that the functions in 3D and 2D have a similar qualitative structure, with 2D leading to a stronger suppression. In 1D, the divergence of the Coulomb potential was suppressed with a cusp-type cutoff set by the parameter x_0. We see that as x_0 approaches zero, $s(k)$ also approaches zero for all k, confirming that the bare Coulomb potential in 1D is impenetrable. However, in order for $s(k)$ to truly approach zero, exceedingly small values of x_0 are required; we see that $s(k)$ still has significant nonzero values even if x_0 is as small as $10^{-8} a^*$, illustrating that true one-dimensional systems, for which $s(k) = 0$ should be rigorously zero for all k, are essentially unattainable. For $x_0 = 10^{-3} a^*$, we find that $s(k)$ has a similar magnitude as in 2D and 3D; however, the behavior at small k is distinctly different for 1D, and we will see that this impacts the temperature dependence.

The attractive Sommerfeld parameter [figure 1(b)] leads to an enhancement of recombination in 2D and 3D. In contrast, in 1D, the Sommerfeld parameter is still suppressive. We see that the divergence at small k in 3D is softened into a plateau in 2D. Again in all cases, $s(k \to \infty) = 1$ as expected.

In the context of trap-assisted recombination, the temperature-dependent Sommerfeld parameter is more relevant. The numerically integrated Sommerfeld parameter is shown in figure 2 for realistic materials parameters ($m^* = 0.1$ and $\epsilon_r = 10$) as a function of temperature. We see that the qualitative conclusions from

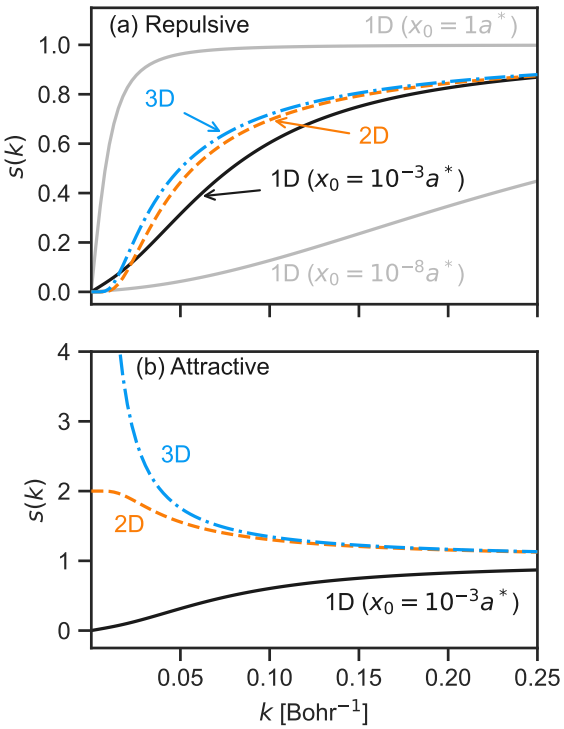

Figure 1. (a) Repulsive and (b) attractive Sommerfeld parameter for $m^* = 0.1$ and $\epsilon_r = 10$ as a function of momentum k. The blue dashed-dotted line corresponds to 3D. The orange dashed line corresponds to 2D. The grey solid lines and the black line correspond to different choices of the cutoff parameter x_0 in 1D.

the analysis of the momentum dependence hold true. For the repulsive interaction [figure 2(a)], a suppression is observed across all temperatures. The low-temperature behavior in 1D differs from the 2D and 3D cases. The true-1D case would give $s(T) = 0$; finite values occur only because of the introduction of a cusp-type cutoff to the Coulomb potential. Smaller x_0 values lead to lower values of $s(T)$. For a given x_0, the suppression of these finite values at low T is less pronounced in 1D than in 2D or 3D. While the exact numerical values depend on the choice of the modified potential, these qualitative conclusions are unaffected.

For the attractive interaction [figure 2(b)], the effects of dimensionality are more pronounced. We see that in 3D, a divergent enhancement is obtained at low temperatures. In 2D, the Sommerfeld parameter leads to an enhancement ($s = 2$) but is effectively independent of temperature. In 1D, even an attractive potential leads to a suppression ($s < 1$), and $s(T)$ decreases at low temperature.

In 3D and 2D, an analytical form for the temperature-dependent Sommerfeld parameter (Eqs. 16 and 29, respectively) was obtained. However, the derivation relied on approximations to simplify the expressions: it has been shown that these approximations may not be strictly valid over the range of temperatures where they are employed [12]. The relative error of the analytical expressions compared to direct

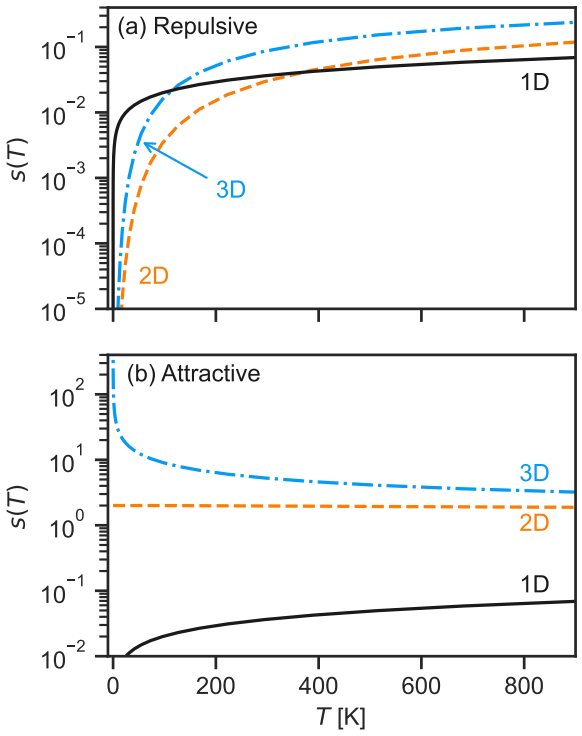

Figure 2. (a) Repulsive and (b) attractive Sommerfeld parameter for $m^* = 0.1$ and $\epsilon_r = 10$ as a function of temperature T. The blue dashed-dotted line corresponds to 3D. The orange dashed line corresponds to 2D. The black solid line corresponds to 1D with $x_0 = 10^{-3}a^*$.

numerical evaluation is shown in figure 3. We find that the error is comparable for the attractive interaction in 3D and 2D. The error is most severe for the repulsive interaction in 3D. For the repulsive interaction in 2D, a fortuitous cancellation between the assumption that k is small ($k \ll 2\pi|Z|/a^*$) and the use of Laplace's method leads to a marked decrease in the relative error. Still, since most applications of the Sommerfeld parameter rely on numerical results, there is no particular need to use the approximation and we recommend utilizing the numerical evaluation of the temperature dependence to avoid spurious errors.

In our derivation, we assumed an isotropic, non-degenerate band extremum at the Γ point. These assumptions do not affect the generality of our results. When anisotropy is present, we recommend choosing an appropriately averaged effective mass with the derived equations to account for this effect. In materials where the band extremum does not occur at the Γ point, there will be a valley degeneracy that needs to be accounted for. Furthermore, there may be orbital degeneracy. In most cases, degeneracy can simply be handled by including a multiplicative factor and retaining the same functional form of the Sommerfeld parameter derived here. We have implicitly assumed that screening effects are negligible and do not lead to substantial deviations from the ideal $1/r$ behavior at large distances [2]. This assumption is

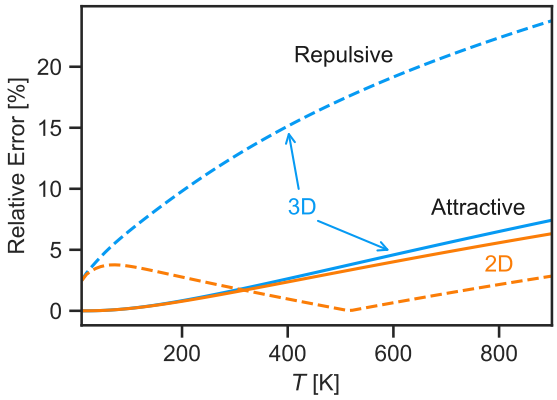

Figure 3. Relative error of the analytical expression (Eqs. 18 and 31) compared to direct numerical evaluation (Eqs. 16 and 29) of the temperature-dependent Sommerfeld parameter. The blue lines correspond to 3D, and orange lines correspond to 2D. Solid lines are for the attractive interaction, dashed lines for the repulsive interaction. Here we utilize $m^* = 0.1$ and $\epsilon_r = 10$.

consistent with low to modest carrier densities. Furthermore, this means that we do not attempt to address 2D electron or hole gases, which have much higher carrier densities. We also assume dilute defect concentrations, for which the overlap of the Coulomb potential can be neglected.

The developments detailed here have now been added to the Nonrad code [25, 12] in version 1.2. When treating trap-assisted recombination in lower dimensions, there may be effects beyond just the Sommerfeld parameter, such as quantum confinement, strain, or nonidealities at the surface or interface. These are best handled within the recombination rate evaluation (e.g., by changing the input parameters that enter the Nonrad code).

4. Implications

Our results clearly show that decreased dimensionality suppresses trap-assisted recombination. The effect is most clear in the attractive interaction: While both 3D and 2D result in an enhancement, the enhancement in 2D can be far less than that of 3D and is independent of temperature. For example, the Sommerfeld parameter takes a value of 44.5 at 4 K and 5.2 at 300 K in 3D when $\epsilon_r = 10$ and $m^* = 0.1$. This is compared to a value of 2 for 2D, independent of temperature. In 1D, an enhancement is no longer possible, only a suppression; we obtain a value of 0.004 at 4 K and 0.04 at 300 K for the same ϵ_r and m^* when $x_0 = 10^{-3}a^*$.

The Sommerfeld parameters do not strongly depend on ϵ_r and m^*, for values of these parameters that are typical for semiconductors and insulators. The Sommerfeld parameter becomes less important [i.e., $s(T)$ approaches 1] as $\epsilon_r \to \infty$ or $m^* \to 0$. Indeed, larger values of ϵ_r correspond to increased screening of the potential, and for smaller values of m^* , the particle moves faster at a given temperature and is less subject to the effects of the potential.

These results have important implications for the physics of real materials and

their applications. Optoelectronic devices commonly employ quantum-well structures, layers of material that can be as thin as a few unit cells, sandwiched between layers of a material with a larger band gap, effectively confining the carriers in the quantum well. The trend to reduce device dimensions in electronics also leads to situations where carriers behave as if confined in 2D or 1D. Our results indicate that the decreasing the dimensionality leads to a reduction in trap-assisted recombination. Notably, the temperature dependence in 3D and 2D is different: experiments that probe low-temperature trap-assisted recombination rates should be able to discern whether dimensionality is playing a role.

Another area in which the dimensionality clearly plays a role is in two-dimensional materials, which are candidates for electronic device applications thanks in part to the ability to construct van der Waals heterostructures [18]. Our results point out an additional benefit of such devices: trap-assisted recombination will be suppressed compared to their bulk counterparts. Two-dimensional materials are also promising as hosts for quantum defects [19, 20, 21, 49, 50, 51, 52]; for example, a single defect embedded in a monolayer of material can be used as a quantum sensor with superior resolution. Carrier trapping at a defect can ruin its quantum properties; the suppression provided by the Sommerfeld parameter could mitigate this process in a 2D material. Going further, even one-dimensional materials, such as nanotubes, are being considered as hosts for quantum defects [23, 24]; they would further benefit from the suppression provided by the Sommerfeld parameter.

5. Conclusions

In conclusion, we have examined the effect of dimensionality on trap-assisted recombination through the Sommerfeld parameter. We derived the temperature-dependent Sommerfeld parameter in 2D and 1D, and obtained an approximate analytical expression in 2D. In 1D, the bare Coulomb potential leads to an identically zero Sommerfeld parameter; a more realistic description was presented by introducing a cusp-type cutoff of the potential. Overall we find that a lowering of dimensionality reduces trap-assisted recombination. This effect is most obvious for an attractive interaction: in 3D, the Sommerfeld parameter leads to an enhancement of trap-assisted recombination; this enhancement is reduced in 2D, while in 1D, a suppression occurs (even when using the cutoff of the Coulomb potential). The formulas derived in this work have now been implemented in the latest version of the Nonrad code [25, 12].

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