Fermion space charge in narrow band-gap semiconductors, Weyl semimetals, and around highly charged nuclei

Eugene B. Kolomeisky,[1] Joseph P. Straley,[2] and Hussain Zaidi[1]
[1]*Department of Physics, University of Virginia, P. O. Box 400714, Charlottesville, Virginia 22904-4714, USA*
[2]*Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506-0055, USA*
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The field of charged impurities in narrow band-gap semiconductors and Weyl semimetals can create electron-hole pairs when the total charge Ze of the impurity exceeds a value $Z_c e$. The particles of one charge escape to infinity, leaving a screening space charge. The result is that the observable dimensionless impurity charge Q_∞ is less than Z but greater than Z_c. There is a corresponding effect for nuclei with $Z > Z_c \approx 170$, however, in the condensed matter setting we find $Z_c \simeq 10$. Thomas-Fermi theory indicates that $Q_\infty = 0$ for the Weyl semimetal, but we argue that this is a defect of the theory. For the case of a highly-charged recombination center in a narrow band-gap semiconductor (or of a supercharged nucleus), the observable charge takes on a nearly universal value. In Weyl semimetals, the observable charge takes on the universal value $Q_\infty = Z_c$ set by the reciprocal of material's fine structure constant.

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I. INTRODUCTION

The experimental success of quantum electrodynamics (QED) lies in the domain of small fields where observations impressively match the theoretical calculations based on perturbation theory in the fine structure constant $\alpha = e^2/\hbar c$. In calculations involving bound states of a nucleus of charge Ze, the fine structure α constant additionally appears in the combination $Z\alpha$. Even though α is small, $Z\alpha$ may not be, so that perturbative analysis can fail when $Z\alpha \gtrsim 1$. One of the most profound physical effects predicted to take place in this regime is the instability of the ground state (the vacuum) against creation of electron-positron pairs, resulting in a screening space charge of electrons with positrons leaving physical picture.[1] Experimental study of this effect has not been possible, as stable nuclei with $Z \gtrsim 1/\alpha \approx 137$ have not been created, and attempts to look for positron production in a temporarily created overcritical system of slowly colliding uranium nuclei have not been successful.[1]

The goal of this paper is to demonstrate that in the condensed matter setting the corresponding problems are the impurity states in narrow band-gap semiconductors (NBGS)[2] and Weyl semimetals (WS).[3] The advantage of these systems is that the charges and fields required to see the ground state instability are modest and readily achievable. Some of the effects may have already been seen[2] without fully appreciating what they represent. The outline of this paper is as follows. In Sec. II, the phenomenon of critical charge is first explained heuristically (IIA) followed by more precise semiclassical argument (IIB) that relates the effect to that of quantum-mechanical fall to the center.[4] Then the critical charge problem for the Coulomb potential modified at small distances is analyzed via dimensional analysis (IIC), which in Sec. III is employed to demonstrate the feasibility of observation of its condensed matter analog, instability with respect to creation of electron-hole pairs in semiconductors.

In Sec. IV, Thomas-Fermi (TF) theory of screening by space charge is derived and its deficiencies and a modification are discussed. One of the byproducts of the analysis is the conclusion that the observable charge of an arbitrary overcritical source in the WS case is always given by the reciprocal of the inverse fine structure constant for the material.

In Secs. V and VI, the TF theory is solved in two steps—uniformly charged half-space → spherically symmetric charge distribution—so that the existence of several physically different regimes of screening can be appreciated, and to establish a relationship with previous analysis.[5,6] The TF analysis leads to the conclusion that there is total screening in the WS case, through an argument that is parallel to Landau's "zero charge effect" in QED.[7] This would have readily observable consequences. However, we will argue in Sec. VII that this claim of complete screening is not right, so that there after all can be an observable charge.

II. CRITICAL CHARGE IN QUANTUM ELECTRODYNAMICS

The Dirac equation for an electron in vacuum in the field of a point charge Ze (the Dirac-Kepler problem) becomes invalid for $Z > 1/\alpha \approx 137$.[7]

A. Heuristic argument

This feature can be heuristically understood by starting with the classical expression for the energy of an electron of mass m_e and momentum p in the field of charge Ze,

$$\varepsilon = c\sqrt{p^2 + m_e^2 c^2} - \frac{Ze^2}{r}, \qquad (1)$$

and trying to estimate the ground-state energy. Since the electron position cannot be determined to better than $\hbar$ divided by the uncertainty of momentum, p and $r \gtrsim \hbar/p$ entering Eq. (1) may be regarded as the typical momentum and size of the quantum state, respectively. Then the state energy can be estimated as

$$\varepsilon(p) \gtrsim c\left(\sqrt{p^2 + m_e^2 c^2} - zp\right), \quad z = Z\alpha, \qquad (2)$$

where z measures the nuclear charge in units of the reciprocal of the fine structure constant $1/\alpha$; both these "natural" units (lower case letters) and the usual units for charge (upper case

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letters) will be used throughout this paper. Minimizing with respect to the free parameter p, we find

$$p_0 \simeq \frac{m_e c z}{\sqrt{1-z^2}}, \quad r_0 \simeq \frac{\hbar}{p_0} \simeq \lambda \frac{\sqrt{1-z^2}}{z}, \quad \lambda = \frac{\hbar}{m_e c} = \frac{r_e}{\alpha}, \tag{3}$$

where λ is the electron Compton wavelength that sets the scale for the uncertainty of measurement of the electron position and $r_e = e^2/m_e c^2$ is the classical electron radius. The lowest (ground-state) energy is then

$$\varepsilon_0 = m_e c^2 \sqrt{1-z^2}. \tag{4}$$

While reproducing the well-known ground-state properties of a hydrogenlike atom in the nonrelativistic $z \ll 1$ limit (3), as well as (coincidentally) matching the exact expression for the ground-state energy (4) based on the analysis of the Dirac equation,[7] these arguments also predict that the minimum of (2) only exists for $z < 1$ ($Z < 137$). As $z \to 1 - 0$, the ground state becomes sharply localized ($r_0 \to 0$), the typical electron momentum diverges ($p_0 \to \infty$), and the ground-state energy vanishes ($\varepsilon_0 \to 0$). The conclusions (3) and (4) become meaningless for $z > z_c = 1$; specifically the ground-state energy is predicted to become imaginary. The counterintuitive independence of z_c of the electron mass m_e can be explained via dimensional analysis:

The Dirac-Kepler problem is fully specified by the dimensionless parameter z, and by the electron Compton wavelength λ in (3). If there exists a critical value of the charge z_c, it can only be a function of the remaining independent dimensionless parameters of the problem. However, having only one length scale λ available makes it impossible to use it in a dimensionless combination. Therefore z_c cannot depend on λ, and thus on the electron mass m_e; the only possible outcome is $z_c \simeq 1$.

These observations imply that the $z > 1$ anomaly of the Dirac-Kepler problem persists in the Weyl-Kepler problem ($m_e = 0$), where the estimate (2) becomes

$$\varepsilon'(p) \simeq pc(1-z). \tag{5}$$

As a result, a charged Weyl fermion placed in the field of a point charge with $z < 1$ is always delocalized ($p_0 = 0$, $r_0 = \infty$, and $\varepsilon_0 = 0$); the spectrum is not discrete (i.e., no bound states). On the other hand, a sufficiently attractive charge $z > 1$ leads to a sharply localized ground state ($p_0 = \infty$, $r_0 = 0$, and $\varepsilon_0 = -\infty$).

The $z > 1$ instability in the Dirac-Kepler problem can be identified with a strong field limit of the Schwinger effect:[8] the creation of electron-positron pairs in vacuum in a uniform electric field. The phenomenon is characterized by the Schwinger typical electric field E_S for which the work to separate the constituents of the electron-positron pair over the length scale of the Compton wavelength is equal to the rest energy of the pair: $eE_S\lambda \simeq m_e c^2$,

$$E_S = \frac{m_e^2 c^3}{e\hbar}. \tag{6}$$

For $E \lesssim E_S$, the pairs are created by tunneling with the vacuum being in a metastable state while for $E \gtrsim E_S$, the vacuum is absolutely unstable with respect to pair creation. For the Coulomb problem, the instability sets in when the electric field of the nucleus a Compton wavelength away from its center, Ze/λ^2, reaches the order of magnitude of the Schwinger field (6), thus predicting $z_c \simeq 1$. In view of its mass independence, the prediction $z_c \simeq 1$ also applies to the Weyl-Kepler problem.

B. Critical charge as a consequence of quantum-mechanical "fall to the center"

The $z > 1$ anomaly of the Dirac equation is related to the "fall to the center" effect of quantum mechanics.[4] For a classical electron of energy $\mathcal{E}$ and angular momentum M moving in a central field $U(r)$, the equation of conservation of energy can be written as

$$p_r^2 = 2m_e E - 2m_e U(r) - \frac{M^2}{r^2} > 0, \tag{7}$$

where $p^2 = p_r^2 + M^2/r^2$ is the square of total momentum and p_r is the radial component of the momentum. The particle can reach the origin (fall to the center) if[9]

$$\lim_{r\to 0}(r^2 U(r)) < -\frac{M^2}{2m_e}. \tag{8}$$

Specifically, for zero angular momentum M, the fall to the center occurs for any attractive potential decreasing faster than $1/r^2$ as $r \to 0$. In quantum mechanics, M^2 has to be replaced by the eigenvalues of the square of the angular momentum operator, which will be chosen in the semiclassical Langer form $M^2 \to \hbar^2(l + 1/2)^2$ in Refs. 1 and 4 so that both the effects of zero-point motion ($l = 0$) and angular momentum ($l \neq 0$) are accounted for. The smallest value of M^2 is $\hbar^2/4$, which implies that the fall to the center can occur for $1/r^2$ potentials that are more attractive than the critical potential satisfying[4]

$$U_c(r \to 0) = -\frac{\hbar^2}{8m_e r^2}. \tag{9}$$

When this condition is met there is no lower bound on the spectrum.

For relativistic classical particle moving in a central field, energy, and momentum are related by $\mathcal{E} = c\sqrt{p_r^2 + M^2/r^2 + m_e^2 c^2} + U(r)$. For bound states, we have $-m_e c^2 < \mathcal{E} < m_e c^2$, where beyond the lower limit the system is unstable against pair creation. At the lower limit the range of motion can be found by solving for the radial momentum to obtain a form analogous to Eq. (7):

$$p_r^2 = \frac{1}{c^2}(U^2(r) + 2m_e c^2 U(r)) - \frac{M^2}{r^2} > 0. \tag{10}$$

If $U(r)$ is diverging as $r \to 0$, the $U^2(r)$ term dominates, and for attractive $U(r)$ the origin can be reached if[10]

$$\lim_{r\to 0}(rU(r)) < -Mc. \tag{11}$$

Classically, the fall to the center for the $M = 0$ state is possible for a potential that at $r \to 0$ is more attractive than a $1/r$ potential. The quantum case is different: substituting in (11) minimal $M^2 = \hbar^{2/}4$, we infer that the fall to the center is possible for $1/r$ potentials more attractive than the critical potential

$$U_c(r \to 0) = -\frac{\hbar c}{2r}. \tag{12}$$

Comparing with the Coulomb field $U = -Ze^2/r$, we deduce $z_c = Z_c\alpha = 1/2$, which is the correct critical charge of the Kepler problem for a spinless particle.[1] It is half the value found for the Dirac particle (the "missing" half is due to the electron spin). The Dirac case cannot be fully understood semiclassically but an insight can be gained by observing that the relativistic case with $\mathcal{E} = -m_e c^2$ is equivalent to a nonrelativistic problem with the effective potential [compare Eqs. (7) and (10)]

$$U_{\rm eff}(r) = -\frac{U^2(r)}{2m_e c^2} - U(r) + \frac{M^2}{2m_e r^2} \tag{13}$$

and zero total energy. We now see that for the Kepler problem, $U(r) = -Ze^2/r$, the particle is *repelled* at large distances. The same effective potential is obtained from the Klein-Gordon equation transformed into the Schrödinger form.[1]

The Dirac equation can be also brought into a Schrödinger form with an effective potential at $\mathcal{E} = -m_e c^2$ resembling Eq. (13) but also exhibiting extra terms attributed to the electron spin.[1] Their role can be (approximately) summarized in a form similar to Eq. (13) with different amplitude of the $1/r^2$ term. Specifically for the Dirac-Kepler problem, we have[1]

$$U_{\rm eff}(r) = \frac{Ze^2}{r} + \frac{\hbar^2(1-z^2)}{2m_e r^2}. \tag{14}$$

We see that the fall to the center occurs for $z > 1$ and then the particle is confined to the central region of radius

$$R_{\rm cl} = \frac{\lambda(z^2-1)}{2z}. \tag{15}$$

As is the case of the fall to the center problem, proper treatment of the instability of the Dirac equation requires accounting for finite radius a of atomic nucleus that modifies the $1/r$ attraction at short distances and removes the difficulty for $z > 1$.[1] For a nucleus with $Z = Z_c \approx 170$ ($z_c \approx 1.24$), the ground-state energy reaches the boundary of the lower continuum, $\varepsilon_0 = -m_e c^2$.[1] Past that point, the total energy of the production of an electron-positron pair becomes negative and the vacuum becomes unstable with respect to pair creation; the positron repelled by the nucleus escapes to infinity while the electron remains near the nucleus.[1]

C. Dimensional analysis

Many of the conclusions of previous analysis of the critical charge problem that accounted for finite radius a of atomic nucleus[1,11] can be reproduced by a combination of dimensional analysis and simple physical arguments. Indeed, now we have a problem fully specified by independent dimensionless combinations Z, α, and a/λ. Then, if there exists a critical value Z_c, it can only be a function of α and a/λ. The electrostatic potential inside the nucleus has the form $\varphi(r) = (Ze/a)G(r/a)$, where $G(1) = 1$ and $G(0)$ is finite. Then the parameters Z and α appear together in the $z = Z\alpha$ combination. Therefore

$$z_c = f\left(\frac{a}{\lambda}\right) \tag{16}$$

or

$$Z_c = \frac{1}{\alpha} f\left(\frac{a}{\lambda}\right) = \frac{\hbar c}{e^2} f\left(\frac{m_e c a}{\hbar}\right), \tag{17}$$

where $f(y)$ is a function that depends on the shape of the charge distribution within the nucleus. The properties of $f(y)$ can be inferred from the following arguments. (i) For $a = 0$, one has $z_c = 1$, which implies the small argument behavior $f(y \to 0) \to 1$. This additionally means that $z_c = 1$ for $m_e = 0$ for arbitrary a (the Weyl-Kepler problem with cutoff).

(ii) In the classical $\hbar \to 0$ limit, the Planck's constant must drop out of Eq. (17). This translates into the large argument behavior $f(y \to \infty) \simeq y$ with the consequence $z_c \simeq a/\lambda$. This is indeed what is expected on physical grounds: the vacuum becomes unstable when the electron potential energy at the center of the nucleus $-e\varphi(0) + m_e c^2$ reaches the boundary of the lower energy continuum $-m_e c^2$. This argument applied to the uniformly charged ball model of the nucleus predicts $f(y \to \infty) \to 4y/3$. On the other hand, $f(y \to \infty) \to 2y$ for the constant potential ball model of the nucleus.

For ordinary heavy nuclei the nuclear size a depends on Z according to the Fermi formula

$$a = 0.61 r_e Z^{1/3} = 0.61\lambda\alpha^{2/3} z^{1/3}. \tag{18}$$

The critical charge z_c is found by simultaneous solution of Eqs. (16) and (18) for $z = z_c$:

$$z_c = f\left(0.61\alpha^{2/3} z_c^{1/3}\right). \tag{19}$$

The electron Compton wavelength is known to be much larger than the nuclear size which means the argument of the function f in Eq. (19) is much smaller than unity. In this limit, the distinction between different models of nuclear charge distribution disappears thus explaining the nearly model-independent value of z_c close to 1.

To add credibility to dimensional analysis we now show that the latter easily solves the problem of instability of the muon vacuum. Indeed, the muon Compton wavelength has the same order of magnitude as the nuclear size since the muon is more than 200 times heavier than the electron. The solution to the problem is then described by Eq. (17) with the electron mass m_e replaced by the muon mass m_μ. We are now in the large argument limit, $f(y \to \infty) \simeq y$, which determines the critical Z for the muon to be

$$Z_c^{(\mu)} = \frac{z_c^{(\mu)}}{\alpha} \simeq \left(\frac{m_\mu}{m_e}\right)^{3/2} \simeq 3000. \tag{20}$$

These conclusions agree with existing analysis of the problem.[1,11] In fact, we observe that approximating the true $f(y)$ dependence for *all* y by its $y \gg 1$ limit[11]

$$f(y) = \tfrac{4}{3}y + 1.1547, \quad y \gg 1 \tag{21}$$

suffices to quickly estimate the critical charge in the practically relevant case of the uniform density model of the nucleus. In the $y \ll 1$ limit, where this approximation is expected to work poorly, the combination of Eqs. (19) and (21) predicts

$Z_c = 163$, which is close to the accepted value of 170. Inspection of previous results[1,11] shows that, except for a narrow vicinity of $y = 0$, the function $f(y)$ is basically a straight line of the right slope with a larger-than-unity offset. The significance of the linear approximation (21) is that it allows us to reliably estimate the critical charge in the condensed matter setting.

III. CRITICAL CHARGE IN CONDENSED MATTER SETTING

QED's predictions of screening by space charge can be tested in performable experiments involving condensed matter systems, both presently available and those that will become available in the near future. Our primary example is that of NBGS whose physics is known to mimic QED.[1] Excitation of an electron-hole pair is analogous to the creation of an electron-positron pair in QED, with the band gap representing the combined rest energy of the particles. Creation of the electron-hole pairs in the presence of a uniform electric field takes place via Zener tunneling,[12] which is analogous to the Schwinger effect.[8] Our contention is that moderately charged impurity regions in semiconductors can trigger a space charge around them that parallels the effects that would occur in QED for unrealistically large $Z \gtrsim 170$.

The idea that the $Z > 137$ anomaly of the original Dirac-Kepler problem may have observable condensed matter implications is due to Keldysh.[2] In his study of the impurity states in semiconductors Keldysh noted that the effective mass approximation,[13] while successful in describing shallow impurity states, fails to explain deep states whose binding energy is comparable with the band gap. Such states are formed near multicharged impurity centers, vacancies, etc., and they cannot be associated with either conduction or valence bands. The experiment presented another puzzle: some highly charged impurities acted as very efficient recombination centers that managed to trap both electrons and holes but an explanation why that was the case was lacking. Keldysh argued that experimental findings can be explained in a two-band approximation (well obeyed in NBGS of the InSb type) where the low-energy electron (hole) dispersion law is relativistic,[2,14]

$$\varepsilon(\mathbf{p}) = \pm\sqrt{(\Delta/2)^2 + v^2 p^2}. \tag{22}$$

Here, the upper and lower signs correspond to the conduction and valence bands, respectively, $\Delta \equiv 2mv^2$ is the energy band gap that parallels twice the rest energy of a particle of mass m, and v is the velocity of a high-momentum particle analogous to the speed of light c. Compared to their vacuum electron-positron counterparts, electrons and holes in NBGS have two orders of magnitude smaller effective mass ($m \simeq 0.01 m_e$) and limiting velocity v nearly three orders of magnitude smaller than the speed of light ($v \approx 4.3 \times 10^{-3} c$). As a result their band gap $\Delta \simeq 0.1$ eV is seven orders of magnitude smaller than the rest energy of the electron-positron pair.[15] Due to these parameter values the analog of large field QED effects are readily realizable in NBGS.

With this in mind, the determination of the impurity states reduces to solving the Dirac equation for a particle of mass m in the field of a charge Ze screened by the dielectric constant ϵ of the semiconductor. In view of the peculiarity of the Dirac-Kepler problem (now $\alpha = e^2/\hbar v\epsilon$), Keldysh argued that for $z = Z\alpha < 1$ the impurity states are given by the known solution to the Dirac equation[7] while the $z > 1$ case with "collapsed" ground state describes a recombination center.

An expression for the NBGS critical charge can be written in a form that parallels Eq. (16):

$$z_c = f\left(\frac{a}{\Lambda}\right), \quad \Lambda = \frac{\hbar}{mv} = \frac{2\hbar v}{\Delta} = \frac{R_e}{\alpha}, \tag{23}$$

where now a is the radius of the impurity region, Λ is the semiconductor analog of the electron Compton wavelength and $R_e = 2e^2/\epsilon\Delta$ is the semiconductor counterpart of the classical electron radius (defined as band electron's delocalization size at which its potential self-energy $e^2/\epsilon R_e$ matches its rest energy $mv^2 = \Delta/2$. We note that since both $R_e \simeq 1$ nm and $\Lambda \simeq 10$ nm significantly exceed the lattice spacing, macroscopic theory of impurity states ignoring the lattice structure of the material suffices.

The density of nuclear matter is known to have the order of magnitude set by the classical electron radius r_e [see Eq. (18)]. It will be made clear shortly, that the large field effects in NBGS become prominent at impurity charge densities set by the NBGS electron radius R_e. Therefore the relationship between the radius a and the charge Z of a uniformly charged region will be chosen as

$$a = 1.3 R_e Z^{1/3} = 1.3\Lambda\alpha^{2/3} z^{1/3} \tag{24}$$

that parallels its nuclear physics counterpart (18); the numerical factor corresponds to the charge density $n_{\text{ext}} = 10^{20}\text{cm}^{-3}$ to be justified below. The NBGS critical charge can be determined by solving the equation

$$z_c = f\left(1.3\alpha^{2/3} z_c^{1/3}\right), \tag{25}$$

this is nearly identical to its QED counterpart (19). Because the value of the limiting velocity v is known, the semiconductor equivalent of the fine structure constant is $\alpha = e^2/\epsilon\hbar v \approx 1.7/\epsilon = 0.17$, an order of magnitude larger than its QED counterpart (we employed $\epsilon = 10$[16]). With this value of α and choosing the function $f(y)$ in the simple form (21), the solution to Eq. (25) is $z_c \approx 1.7$, which implies $Z_c \approx 10$. The corresponding critical cluster size is $a_c \approx 3$ nm according to Eq. (24). Surely, $Z \gtrsim 10$ impurity clusters with sizes in excess of several nanometers are more common objects than $Z \gtrsim 170$ nuclei.

In addition to making it possible to study the regime of large effective fine structure constant, condensed matter systems also offer possibilities that cannot be realized in QED. Indeed, over forty years ago Abrikosov and Beneslavskiĭ[3] predicted the existence of WS having points in the Brillouin zone where the valence and conduction bands meet with a dispersion law that is linear in the momentum. This is the $\Delta = 0$ case of Eq. (22). The low-energy excitations in WS (realizing massless versions of QED) are described by the Weyl equation. We already know that the critical charge for the Weyl-Kepler problem is $z_c = 1$. Equation (5) additionally implies lack of the discrete spectrum for $z < 1$; for $z > 1$, a space charge of Weyl fermions is present in the ground state. Such substances are likely to be realized in doped silver chalcogenides $Ag_{2+\delta}Se$ and $Ag_{2+\delta}Te$,[17] pyrochlore iridates $\mathcal{A}_2Ir_2O_7$ (where $\mathcal{A}$ is yttrium or a lanthanide),[18] and in topological insulator multilayer structures.[19] The zero energy gap of WS implies that in a *uniform* electric field the creation of a space charge of Weyl fermions is spontaneous. The dielectric constant of WS is of order 10 with $e^2/\hbar v \simeq 1$,[3] thus leading, like in the NBGS case, to $Z_c \simeq 10$ independent of the size of the impurity region.

NBGS and WS are condensed matter systems where analogs of the atomic collapse of QED can be experimentally detected. Related phenomena can be also observed in graphene. Indeed, graphene possesses the linear dispersion law analogous to that of WS and microscopic parameters similar to NBGS which leads to a small value for the critical charge for promotion of electrons from the valence band to the conduction band. Such a problem has been considered elsewhere[20] and experimental signatures of the "atomic collapse" in graphene were recently reported.[21] The graphene problem is mathematically different from what we discuss, because graphene is a two-dimensional semimetal embedded in a three-dimensional space.

Below, we will determine the ground-state properties of NBGS and WS in the presence of a finite-size positive Coulomb impurity (a negative charge leads to the same discussion due to particle-hole symmetry). The arguments given above imply that at modest Z electrons are promoted from the valence band to form a space charge around the impurity while the holes leave the physical picture; the properties of the space charge vary with Z and α and are determined by the interplay of attraction to the impurity (promoting the creation of electron-hole pairs), and electron-electron repulsion combined with the Pauli principle (limiting the creation of the space charge). The QED analysis of the physical properties of the space charge was carried out in two limits: (i) Z close to Z_c, where there are very few electrons promoted to the conduction band for which the single-particle picture is a good starting point;[1] and (ii) $Z \gg Z_c$, where the number of screening electrons is large and the electron-electron interactions cannot be ignored.[5,6]

Below we demonstrate that the physics in the $Z \gg Z_c$ limit exhibits a large degree of universality. Although we are mostly concerned with the NBGS setting, our findings are equally applicable in QED as both problems share the same mathematics; a solution to the WS problem benefits the understanding of the NBGS/QED case.

To help the readers orient themselves between three physically different manifestations of the problem and to provide them with a condensed matter-QED translation dictionary, in Table I, we summarized pertinent properties of electrons in vacua of QED, NBGS, and WS. The entries not yet specified are (i) *the fermion degeneracy factor* g, which is 2 in QED, while in NBGS it is twice the number of Dirac valleys (22) within the first Brillouin zone; an isotropic valley-independent limiting velocity v is assumed for simplicity. In the WS case, g counts the number of Weyl points within the first Brillouin zone: $g = 24$ in pyrochlore iridates[18] and $g = 2$ in a topological insulator multilayer.[19] (ii) *The coupling constant* γ plays a role analogous to that of the fine structure constant α in polarization effects, as will be made clear below. (iii) *The Zener field* E_Z is the semiconductor analog of the Schwinger field (6) defined as

$$E_Z = \frac{\Delta^2}{e\hbar v}. \tag{26}$$

TABLE I. Summary of properties of electrons in vacua of quantum electrodynamics (QED), narrow band-gap semiconductors (NBGS), and Weyl semimetals (WS).

Media	QED	NBGS	WS
Electrons	free	band Dirac	band Weyl
Mass	m_e	$m \simeq 10^{-2} m_e$	0
Degeneracy g	2	$\geqslant 2$	$\geqslant 2$
Dielectric constant	$\epsilon = 1$	$\epsilon \approx 10$	$\epsilon \simeq 10$
Limiting speed	c	$v \approx 4 \times 10^{-3} c$	$v \simeq 10^{-2} c$
Band gap or rest energy	$2 m_e c^2$	$10^{-7} \times 2 m_e c^2$	0
Fine structure constant α	$\frac{e^2}{\hbar c} \approx \frac{1}{137}$	$\frac{e^2}{\hbar v \epsilon} \approx \frac{1}{6}$	$\frac{e^2}{\hbar v \epsilon} \simeq 0.1$
Coupling constant γ	$\frac{4\alpha^3}{3\pi} \approx 10^{-7}$	$\frac{2g\alpha^3}{3\pi} \lesssim 10^{-3}$	$\frac{2g\alpha^3}{3\pi} \lesssim 10^{-3}$
Classical radius of electron	$r_e \simeq 10^{-6}$ nm	$R_e \simeq 1$ nm	∞
Compton wavelength	$\lambda \simeq 10^{-4}$ nm	$\Lambda \simeq 10$ nm	∞
Schwinger or Zener field	$E_S \simeq 10^{16}\ \frac{\mathrm{V}}{\mathrm{cm}}$	$E_Z \simeq 10^{5}\ \frac{\mathrm{V}}{\mathrm{cm}}$	0

Comparing the values of the fields E_S and E_Z explains why NBGS are so well suited to study strong field QED effects; the situation is even more favorable in WS where due to the zero band gap, an arbitrarily weak field is "strong" as far as the space charge phenomena are concerned.

IV. THOMAS-FERMI THEORY

Since for $Z \gg Z_c$ a large number of electrons are in the conduction band, the properties of the system consisting of the impurity and its interacting cloud of electrons can be understood semiclassically with the help of the TF theory.[5,6] The main object of the latter is a physical electrostatic potential $\varphi(\mathbf{r})$ felt by an electron that is due to both the electrostatic potential of the impurity $\varphi_{\text{ext}}(\mathbf{r})$ and that of the space charge characterized by the number density $n(\mathbf{r})$:

$$\varphi(\mathbf{r}) = \varphi_{\text{ext}}(\mathbf{r}) - \frac{e}{\epsilon} \int \frac{n(\mathbf{r}')dV'}{|\mathbf{r} - \mathbf{r}'|}. \tag{27}$$

The external potential $\varphi_{\text{ext}}(\mathbf{r})$ is a pseudopotential that represents the perturbation of the system caused by the impurity; even though φ_{ext} is not entirely of electrostatic origin, we will define $\Delta\varphi_{\text{ext}} = -4\pi e n_{\text{ext}}/\epsilon$. We assume that the impurity charge density $e n_{\text{ext}}(\mathbf{r})$ is spherically symmetric and localized within a mesoscopic region of size a so that for $r \geqslant a$ the potential $\varphi_{\text{ext}}(\mathbf{r})$ reduces to a purely Coulomb form $\varphi_{\text{ext}}(r) = Ze/\epsilon r$ of a net charge Ze. There are several reasons why the impurity region has to be mesoscopic in size. First of all, in practice charged atomic scale defects cannot have $Z \gtrsim 10$. Second, a large charge localized within a small region implies a large electrostatic potential. However, all our analysis is based on approximating the exact dispersion law by its low-energy limit (22). For that to remain valid, the order of magnitude of the potential within the impurity region should not exceed a volt. Like in graphene, this corresponds to the electron volt energy scale, which is significantly smaller than the width of the conduction band. Finally, the conditions of semiclassical description inherent within the TF theory must be met. All these constraints along with the requirement $Z \gg Z_c \simeq 10$ can be satisfied in $a \gtrsim 10$ nm impurity clusters. Promotion of electrons to the conduction band also takes place in smaller (down to 3 nm) regions but the number of these electrons may not be large enough for the predictions of the TF theory to be quantitatively reliable.

Given $\varphi(\mathbf{r})$, one can deduce that the electron number density $n(\mathbf{r})$ is different from zero only in the region of space where the electron potential energy $-e\varphi(\mathbf{r}) + \Delta/2$ drops below $-\Delta/2$, thus defining the edge of the space charge region as

$$e\varphi(\mathbf{r}) > \Delta, n(\mathbf{r}) > 0. \qquad (28)$$

The radius of the space charge region $R_{sc} \geqslant a$ is given by the equalities $e\varphi(R_{sc}) = \Delta$, $n(R_{sc}) = 0$; outside the region, we have $n = 0$ and

$$\varphi = \frac{Q_\infty e}{\epsilon r}, \quad r > R_{sc} = \frac{1}{2} Q_\infty \frac{2e^2}{\epsilon \Delta} \equiv \frac{1}{2} Q_\infty R_e, \qquad (29)$$

where $Q_\infty < Z$ is the observable charge as seen at large distances from the source center. Continuity of the potential φ across the shell boundary relates R_{sc} and Q_∞, while the NBGS electron radius R_e sets the length scale as indicated in the last two steps in (29) meaning that we can speak of the shell size or the observable charge interchangeably. We note that in the WS case, $R_e = \infty$, Eq. (29) predicts $R_{sc} = \infty$, i.e., the electron shell extends all the way to infinity. In natural units of charge, the relationship between the observable charge $q_\infty = Q_\infty \alpha$ and the radius of the electron shell is given by

$$q_\infty = \frac{2R_{sc}}{\Lambda}. \qquad (30)$$

From the thermodynamical standpoint, creation of electron (e)-hole (h) pairs by the field of a Coulomb impurity accompanied by escape of a hole to infinity may be viewed as a "chemical reaction" $e + h \leftrightarrows 0$ (the ground state of the semiconductor is the "vacuum");[13] the condition of equilibrium for this reaction has the form

$$\mu_e + \mu_h = 0, \quad \mu_e = \sqrt{(\Delta/2)^2 + v^2 p_F^2} - e\varphi, \quad \mu_h = \Delta/2, \qquad (31)$$

where μ_e and μ_h are the chemical potentials of the electrons and holes, respectively, and

$$p_F(\mathbf{r}) = \hbar \left(\frac{6\pi^2 n(\mathbf{r})}{g} \right)^{1/3} \qquad (32)$$

is the Fermi momentum, which we assume is a slowly varying function of position $\mathbf{r}$.

The condition of equilibrium (31) together with Eq. (32) implies a relationship between the physical potential and the number density of the space charge:[5,6]

$$n(\mathbf{r}) = \frac{\gamma}{4\pi} \left\{ \frac{\epsilon \varphi(\mathbf{r})}{e} \frac{\epsilon}{e^2} [e\varphi(\mathbf{r}) - \Delta] \right\}^{3/2}, \qquad (33)$$

where

$$\gamma = \frac{2g\alpha^3}{3\pi} \qquad (34)$$

is the coupling constant characterizing the relative strength of electron-electron interactions and zero-point motion. The four orders of magnitude disparity between its condensed matter and QED values (see Table I) is yet another indication that the space charge phenomenon is more relevant to semiconductors than to QED.

Since the electron chemical potential in (31) is set at the boundary of the lower continuum, in the NBGS/QED cases the screening of the external charge is incomplete; only in the WS ($\Delta = 0$) case we have complete screening. The latter statement can be rigorously proven by setting $\Delta = 0$ in (31) and combining the outcome with Eqs. (27) and (32):

$$\left(\frac{4\pi n(\mathbf{r})}{\gamma} \right)^{1/3} - \frac{\epsilon \varphi_{ext}(\mathbf{r})}{e} + \int \frac{n(\mathbf{r}')dV'}{|\mathbf{r} - \mathbf{r}'|} = 0. \qquad (35)$$

Taking in Eq. (35) the $r \to \infty$ limit gives a relationship

$$\int n(\mathbf{r})dV = Z \left[1 - \lim_{r \to \infty} \left(\frac{4\pi n(\mathbf{r}) r^3}{\gamma Z^3} \right)^{\frac{1}{3}} \right], \qquad (36)$$

whose consequences are that the electron number density $n(\mathbf{r})$ must decay faster than r^{-3} at r large and that

$$\int n(\mathbf{r})dV = Z, \qquad (37)$$

i.e., according to TF theory, a WS succeeds in giving complete screening of the impurity charge.

Applying the Laplacian operator to both sides of Eq. (27) and using (33), we find the relativistic TF equation

$$\nabla^2 \left(\frac{\epsilon \varphi}{e} \right) = -4\pi n_{ext} + \gamma \left[\frac{\epsilon \varphi}{e} \frac{\epsilon}{e^2} (e\varphi - \Delta) \right]^{3/2}, \qquad (38)$$

which was investigated in QED for the case of localized source term.[5,6]

Applicability of the zero-temperature TF theory to experiments to be conducted at finite temperature requires further justification. Since the 0.1 eV energy gap of NBGS significantly exceeds the room-temperature scale of 1/40 eV, the zero temperature theory adequately describes room-temperature experiments. However, WS have a zero-energy gap and in equilibrium the conduction and valence bands are populated with electrons and holes, respectively. This effect can be also neglected as we are working at a potential close to 1 V, significantly exceeding the room-temperature energy scale.

A. Range of applicability of the Thomas-Fermi theory and proposal for its improvement

In order to establish the range of applicability of the TF theory, we note that the observable charge q_∞ is the critical charge of the single-particle problem for a charged region of scale R_{sc}, which is due to both the external charge and that of the space charge. Then replacing $a \to R_{sc}$ in Eq. (23), we arrive at the definition

$$q_\infty = f\left(\frac{R_{sc}}{\Lambda} \right), \qquad (39)$$

which is consistent with the TF result (30) only in the classical limit $R_{sc} \gg \Lambda$ [recall that $f(y \to \infty) \simeq y$, Sec. II]. However, WS are characterized by $\Lambda = \infty$ and so the semiclassical condition can never be met. The consequence is that the prediction of complete screening in the WS case, $q_\infty = Q_\infty \alpha = 0$, an exact consequence of the TF theory, is an artifact. In reality, the WS will screen an overcritical impurity charge by space charge only until the point at which the single-particle description is restored. This sets a limit on the applicability of the TF theory to the WS case at large distances from the source center and implies that the space charge region has a finite radius to be estimated below.

Since the Weyl-Kepler problem with $z < 1$ does not have a discrete spectrum, Coulomb impurities in WS can never be fully neutralized. Their observable charge q_∞ is either 1 (and then there is a space charge of Weyl electrons) or $z < 1$ (when there is no space charge).

More generally, Eq. (39) implies that in the NBGS/QED setting the screening is never so great (in the case $z > z_c$) that the observable charge q_∞ is less than unity. In the point charge limit $a \to 0$, the space charge region must also shrink to a point ($R_{\rm sc} \to 0$), and then Eq. (39) predicts $q_\infty = 1$, i.e., disallowance for a point charge to have observable charge exceeding unity.[5]

Since the Dirac-Kepler problem always has bound states, Coulomb impurities in NBGS can be neutral or ionized with the outer electron shells partially or fully filled with ($Z > Z_c$) or without ($Z < Z_c$) the space charge being present. Here, we only consider the problem of an overcritical $Z > Z_c$ ion with all outer shells empty.

To summarize, the condition of applicability of the TF theory can be stated in two equivalent forms, $R_{\rm sc} \gg \Lambda$ or $q_\infty \gg 1$. Ultimately, the TF treatment of the space charge in the presence of the supercritical source $z \gg z_c$ is applicable because the fine structure constant is significantly smaller than unity.

In order to see what physics is missing from the TF theory, we observe that the relationship between the observable charge and the radius of the electron shell (30) resembles the $z \gg 1$ limit of the semiclassical expression (15) for the localization scale of an electron (replacing $\Lambda \to \lambda$ and $q_\infty \to z$). The latter is sensitive to the fall to the center occurring at $z = 1$ while the TF result (30) is not. The same can be seen more generally by solving the main equation of the TF theory (31) relative to p_F^2:

$$p_F^2 = \frac{1}{v^2}[(e\varphi)^2 - e\varphi\Delta]. \qquad (40)$$

With the identifications $-e\varphi \to U$, $v \to c$, $\Delta \to 2m_e c^2$, this is the energy relationship (10), but the term involving the angular momentum is missing. We propose including this into the right-hand side of Eq. (38):

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d}{dr}\frac{\epsilon\varphi}{e}\right) = -4\pi n_{\rm ext}(r) + \gamma\left[\frac{\epsilon\varphi}{e}\frac{\epsilon}{e^2}(e\varphi - \Delta) - \frac{1}{\alpha^2 r^2}\right]^{3/2}. \qquad (41)$$

At the boundary of the space charge region where the potential is given by Eq. (29), the expression in the second line vanishes leading to a relationship between observable charge q_∞ and the radius of the space charge region $R_{\rm sc}$,

$$q_\infty = \frac{R_{\rm sc}}{\Lambda} + \sqrt{\left(\frac{R_{\rm sc}}{\Lambda}\right)^2 + 1}, \qquad (42)$$

generalizing the TF result (30) and correctly capturing the limiting cases of $R_{\rm sc} \gg \Lambda$ and $R_{\rm sc} \ll \Lambda$. This is equivalent to choosing the function f in (39) in the $f(y) = y + \sqrt{y^2+1}$ form. Assessing the status of our modification of the TF theory (41) requires a separate investigation which we postpone until the future. At the very least, what is proposed qualifies as an interpolation. Until we learn more about the deficiencies of the TF theory, we focus on its standard version accumulated in Eqs. (33) and (38). Some other desirable features of the modified TF equation (41) are mentioned in Sec. VII.

V. STRONG SCREENING REGIME: $\gamma Z^2 \gg 1$

The phenomenon of screening is a manifestation of the electron-electron interactions quantified by the coupling constant γ. Its smallness (see Table I) does not imply that the screening response is necessarily weak. Previous analysis[6] established that the strength of screening is determined by the dimensionless combination γZ^2, which for $Z \gg Z_c$ can take on an arbitrary value. Below we additionally show that in the NBGS/QED cases the regime of strong screening further subdivides into that of superstrong screening $Z \gg \gamma^{-3/2}$ (that is hardly accessible in practice) and the regime of moderately strong screening $\gamma^{-1/2} \ll Z \ll \gamma^{-3/2}$, which is treated in detail.

A. Uniformly charged half-space

Since the source region is mesoscopic in size, we find it useful to start with the problem of screening of a uniformly charged half-space ("half-infinite" nuclear matter in the QED setting) by space charge. This requires solution of the one-dimensional version of Eq. (38):

$$\frac{d^2}{dx^2}\left(\frac{\epsilon\varphi}{e}\right) = -4\pi n_{\rm ext}(x) + \gamma\left[\frac{\epsilon\varphi}{e}\frac{\epsilon}{e^2}(e\varphi - \Delta)\right]^{3/2}, \qquad (43)$$

where $n_{\rm ext}(x < 0) = 3Z/4\pi a^3$, while $n_{\rm ext}(x > 0) = 0$. The solution to Eq. (43) within the source region far away from the boundary $\varphi(x \to -\infty) \equiv \varphi_{-\infty}$ corresponds to the state of local neutrality $n = n_{\rm ext}$:[5]

$$\frac{\epsilon\varphi_{-\infty}}{e}R_e = 1 + \sqrt{1 + \left(\frac{4\pi n_{\rm ext} R_e^3}{\gamma}\right)^{2/3}}. \qquad (44)$$

The quantity $e\varphi_{-\infty}$ is the work function, i.e., the energy needed to remove the electron from the source region. At this point, we observe that in the QED ($R_e \to r_e, n_{\rm ext} r_e^3 \simeq 1, \gamma \ll 1$) and WS ($R_e = \infty$) versions of the problem, Eq. (44) simplifies to

$$\varphi_{-\infty} = \frac{e}{\epsilon}\left(\frac{4\pi n_{\rm ext}}{\gamma}\right)^{1/3}. \qquad (45)$$

In the condensed matter setting, our theory is applicable provided the potential $\varphi_{-\infty}$ does not exceed a volt. Then for $\gamma \simeq 10^{-3}$ and $\epsilon \simeq 10$ the maximal external charge density within the impurity region can be estimated as $n_{\rm ext} \simeq 10^{20}{\rm cm}^{-3}$, two orders of magnitude smaller than the free-electron density in normal metals. This corresponds to $n_{\rm ext} R_e^3 \approx 0.1$ and justifies Eq. (24). With these parameter values the approximation (45) also holds in NBGS. Given the charge concentration of $n_{\rm ext} = 10^{20}{\rm cm}^{-3}$, a 10-nm impurity region would contain a bare charge of about 400 which is significantly larger than $Z_c \approx 10$. Yet larger values of $Z \gg Z_c$ can be obtained by choosing $a \gtrsim 10$ nm: a 20-nm region will host an external charge of about 3000.

The source boundary represents a perturbation to the constant n_{ext}; assuming the effect is weak we substitute $\varphi = \varphi_{-\infty}(1-\phi), 0 \leqslant \phi \ll 1$, into Eq. (38) and linearize about $\varphi = \varphi_{-\infty}$:

$$\frac{d^2\phi}{dx^2} - \kappa^2\phi = 0, \tag{46}$$

where the length scale

$$\kappa^{-1} = 3^{-1/2}(4\pi n_{\text{ext}})^{-1/3}\gamma^{-1/6} = \frac{e}{\sqrt{3\gamma}\varphi_{-\infty}\epsilon} = 3^{-5/6}(\gamma Z^2)^{-1/6}a \simeq R_e\gamma^{-1/6} \tag{47}$$

parallels the Debye length of the TF theory of screening in a Fermi gas;[16] κ^{-1} is the scale over which the potential φ recovers to $\varphi_{-\infty}$ when disturbed by an inhomogeneity. The last estimate in (47) is only applicable to the NBGS or QED ($R_e \to r_e$) cases. In the condensed matter setting with $\gamma \simeq 10^{-3}$, the TF screening length is of the order several nanometers. In QED, κ^{-1} is an order of magnitude larger than the classical electron radius.

Applicability of the concept of the screening length to a finite size system is limited by the constraint $\kappa^{-1} \ll a$ which is a statement of strong screening $\gamma Z^2 \gg 1$.[6] The crossover in the screening response occurs at a charge

$$Z_x \simeq \gamma^{-1/2}. \tag{48}$$

In condensed matter applications, we find $Z_x \simeq 30$; both the regimes of weak $10 \lesssim Z \lesssim 30$ and strong $Z \gtrsim 30$ screening are experimentally accessible. In QED, we have $Z_x \simeq 3000$, which is only of academic interest. Assuming the potential at the impurity boundary is not significantly smaller than $\varphi_{-\infty}$, the $\varphi(x<0)$ dependence can be inferred from the linearized form (46), which gives $\varphi_{-\infty} - \varphi(x<0) \propto e^{\kappa x}$: while local neutrality holds far away from the boundary, it is violated in a boundary layer whose size has the order of magnitude of the TF screening length κ^{-1}.

Outside the impurity region $x > 0$ the potential will continue to decrease from its value at the boundary $\varphi(x=0)$ until it reaches the edge of the space charge region defined as $e\varphi(x = L_{\text{sc}}) = \Delta$. The length scale L_{sc} has a meaning of the thickness of the layer of space charge outside the impurity region.

We thus see that a layer of net positive charge of thickness κ^{-1} localized next to the boundary is followed by a layer of negative charge of thickness L_{sc} outside the source region.[5,6] The net charge of this double layer is positive thus implying that the electric field for $x > L_{\text{sc}}$ is finite and uniform.

Even though Eq. (43) can be integrated in quadratures, an approximate solution is more illuminating. Within the source region the potential is approximated by the solution to Eq. (46) finite at $x = -\infty$:

$$\frac{\epsilon\varphi}{e} = \frac{\epsilon\varphi_{-\infty}}{e}(1-\phi) = \frac{\kappa}{\sqrt{3\gamma}}(1 - Ae^{\kappa x}), \tag{49}$$

where it is assumed (and later justified) that $A \ll 1$.

Outside the impurity region $x > 0$ the full nonlinear equation (43) becomes

$$\frac{d^2}{dx^2}\left(\frac{\epsilon\varphi}{e}\right) = \gamma\left[\frac{\epsilon\varphi}{e}\frac{\epsilon}{e^2}(e\varphi - \Delta)\right]^{3/2}. \tag{50}$$

In the WS case or when $e\varphi \gg \Delta$, Eq. (50) simplifies to

$$\frac{d^2}{dx^2}\left(\frac{\epsilon\varphi}{e}\right) = \gamma\left(\frac{\epsilon\varphi}{e}\right)^3. \tag{51}$$

An analytic solution to the problem of screening of a supercharged nucleus in the strong screening limit $\gamma Z^2 \gg 1$ that approximates the finite nucleus by half-infinite nuclear matter and relies on Eqs. (46) and (51) was proposed by Migdal, Voskresenskiĭ, and Popov (MVP).[6]

For $x > 0$, the solution to Eq. (51) satisfying the conditions of zero electric field and zero potential at $x = \infty$ has the form

$$\frac{\epsilon\varphi}{e} = \sqrt{\frac{2}{\gamma}}\frac{1}{x+B}. \tag{52}$$

Continuity of the potential and of the electric field at the source boundary $x = 0$ determines the integration constants A and B in Eqs. (49) and (52) to be

$$A \approx 0.2374, \quad B = \beta\kappa^{-1} \simeq (\gamma Z^2)^{-1/6}a, \quad \beta \approx 3.212. \tag{53}$$

The length scale B naturally has the order of magnitude of the TF screening length κ^{-1}.

The profile of the electron number density for $x > 0$ is implied by Eqs. (33) and (52):

$$n(x) = \frac{1}{2\pi}\sqrt{\frac{2}{\gamma}}\frac{1}{(x+B)^3}. \tag{54}$$

In the $x \gg B \simeq \kappa^{-1}$ limit, the MVP solution (52) and (54) exhibits universality, i.e., it becomes independent of the parameters of the source region.

B. Spherically-symmetric charge distribution

The MVP solution Eqs. (49)–(54) with $x \to r - a$ is partly relevant to the problem of screening response of NBGS or WS to the spherically symmetric charge distribution of radius a. Specifically, Eq. (49) adequately solves the problem within the impurity region in the strong-screening regime $\gamma Z^2 \gg 1$. For example, the net charge within the source region can be estimated as[6]

$$Q(r \leqslant a) \simeq \kappa^{-1}a^2(Z/a^3) \simeq Z(\gamma Z^2)^{-1/6}. \tag{55}$$

This is significantly smaller than the bare charge Z thus illustrating substantial screening of the source region.

On the other hand, the density profile Eq. (54) with $x \to r - a$ integrates to an infinite charge in three dimensions. Therefore outside a spherically symmetric charge distribution Eqs. (52) and (54) are only applicable as long as approximating the spherical surface by a plane is valid, i.e., for $x = r - a \ll a$. In order to go beyond the limitation of the MVP approximation outside the source region, we need to solve the full three-dimensional equation (38).

1. Weyl semimetal

Outside of the source in the WS ($\Delta = 0$) case, one has to look at the full nonlinear equation (38) whose radially symmetric solution is sought in the form

$$\frac{\epsilon\varphi(r)}{e} = \frac{1}{r}\chi\left(\frac{r}{a}\right), \quad (56)$$

where, via Gauss's theorem, the function χ is related to the charge $Q(r)$ within a sphere of radius r as

$$Q(r) = -r^2\frac{\partial(\epsilon\varphi/e)}{\partial r} = \chi(\ell) - \chi'(\ell), \quad \ell = \ln\frac{r}{a}. \quad (57)$$

Substituting (56) into (38) for $r > a$ and $\Delta = 0$, we obtain the equation

$$\chi''(\ell) - \chi'(\ell) = \gamma\chi^3. \quad (58)$$

For $\ell = \ln(r/a) \ll 1$, we can neglect here the first-order derivative term $\chi'(\ell)$ compared to $\chi''(\ell)$; then $Q(r) \approx -\chi'(\ell)$. The solution to (58) in this limit is the MVP result (52) in disguise

$$\chi_1(\ell) = \sqrt{\frac{2}{\gamma}}\frac{1}{\ell + B/a}, \quad 0 \leqslant \ell \ll 1. \quad (59)$$

In the strong-screening limit $\gamma Z^2 \gg 1$, the parameter $B/a \simeq (\gamma Z^2)^{-1/6}$ drops out of Eq. (59), and the solution to the full Eq. (58) has the form $\chi(\lambda,\ell) = (2/\gamma)^{1/2}y(\ell)$, where $y(\ell)$ is a parameter free universal function satisfying singular boundary condition $y(\ell \to 0) \to \ell^{-1}$. The latter behavior is no longer an accurate representation of the true dependence $y(\ell)$ past $\ell \simeq 1$. Therefore the solution (59) is only applicable up to a crossover scale $\ell = \ell^* \simeq 1$, i.e., within several source radii as was already observed earlier. Within this range, the rescaled potential $\epsilon\varphi/e$ drops from a value of the order $\gamma^{-1/2}(\gamma Z^2)^{1/6}a^{-1}$ at the source boundary to $\gamma^{-1/2}a^{-1}$ at the crossover scale ℓ^*, and the charge within a sphere of radius $r = ae^{\ell}$ drops from the value given by Eq. (55) at the source boundary to $Q^* \simeq -\chi_1'(1) \simeq \gamma^{-1/2}$ at the crossover scale ℓ^*.

For $\ell = \ln(r/a) \gg 1$, we can neglect in Eq. (58) the second-order derivative term $\chi''(\ell)$ compared to $\chi'(\ell)$; then $q(\ell) = Q(r)\alpha \approx \chi(\ell)\alpha$ and for arbitrary screening strength and in natural units of charge, Eq. (58) acquires the form

$$\frac{dq}{d\ell} = -\frac{2g\alpha}{3\pi}q^3, \quad (60)$$

which is mathematically identical to the Gell-Mann-Low (renormalization-group) equation[7] for the physical charge in QED reflecting the effects of vacuum polarization. Equation (60) exhibits the Landau "zero charge" effect:[7] for any "initial" value of q the system "flows" to the zero charge fixed point $q = 0$ as $\ell \to \infty$ ($r \to \infty$), i.e., the source charge has been completely screened. Alternatively, for r fixed complete screening is reached in the point source limit $a \to 0$. Zero observable charge is an exact property of the TF theory discussed in Sec. IV.

In the strong-screening regime, the last equation is applicable at $\ell \gtrsim \ell^* \simeq 1$. As a result, the charge $q(r)$ inside a sphere of radius $r > a^* = ae^{\ell^*} \gtrsim a$ will be given by

$$q^2(r) = \frac{z^{*2}}{1 + (4g\alpha z^{*2}/3\pi)\ln(r/a^*)} \to \frac{3\pi}{4g\alpha\ln(r/a^*)}, \quad (61)$$

where the integration constant $z^* = Q^*\alpha$ is the charge within a sphere of radius a^*. Since $\gamma Q^{*2} \simeq 1$, the constant can be estimated as $z^* \simeq \alpha^{-1/2} \gg 1$ thus implying that the observable charge will be accurately given by the last representation in (61) at distances exceeding several impurity radii. Substituting $Q = q/\alpha = \chi$ into Eqs. (56) and (33), we find corresponding expressions for the potential,

$$\varphi(r) \approx \frac{e}{\epsilon r\sqrt{2\gamma\ln(r/a^*)}} = \frac{e}{2\epsilon r}\sqrt{\frac{3\pi}{g\alpha^3\ln(r/a^*)}}, \quad (62)$$

and the electron density,

$$n(r) \approx \frac{\gamma}{4\pi r^3}\frac{1}{[2\gamma\ln(r/a^*)]^{3/2}} = \frac{1}{16\pi r^3}\sqrt{\frac{3\pi}{g\alpha^3}}\ln^{-3/2}\left(\frac{r}{a^*}\right), \quad (63)$$

both valid for $r \gtrsim a^* \simeq a$. We note that due to the logarithmic factor, the density profile is integrable. This feature, a reflection of the three-dimensional character of the problem, is missing from the MVP result (54).

The hallmark of Eqs. (61)–(63) is their near universality: a weak logarithmic dependence on the source size $a \simeq a^*$ with universal amplitudes. Since both a and a^* appear within arguments of the logarithm, in what follows for simplification purposes the difference between them will be neglected. We conclude that for $\gamma Z^2 \gg 1$ the solution to the screening problem within several impurity radii from the source boundary is universal and given by the MVP results, Eqs. (52) and (54), that turns nearly universal, Eqs. (61)–(63), at larger distances.

We argued previously (see Sec. IV A) that the complete screening effect is an artifact—the observable charge of an overcritical source region must be always equal to unity ($1/\alpha$). Substituting this value into Eq. (61) provides us with a length scale

$$R_W \simeq ae^{3\pi/2g\alpha}, \quad (64)$$

which is the radius of the space charge region: for $r > R_W$ the electron density is negligible and the potential is that of unit ($1/\alpha$) charge. The TF results (61)–(63) are applicable at distances $r \ll R_W$. The exact magnitude of the exponential is explained in Sec. VII.

In QED, the exponential factor in (64) is about 10^{140}. Then R_W is the largest length scale of the problem and for all practical purposes TF theory is exact in the $Z \gg Z_c$ regime.

In WS with $g = 24$ and $\alpha = 1/10$, the exponential factor in (64) is close to 7, which means that the whole spatial structure of the overcritical Weyl ion is experimentally accessible. This system is particularly interesting because both the TF, $r \ll R_W$, and the non-TF, $r \gg R_W$, regions can be probed. On the other hand, choosing $g = 2$ gives the exponential factor of the order 10^{10}, which for a nanometer scale impurity region corresponds to the Weyl ion of 10-m radius. In the latter case, the TF theory provides practically exact description.

2. Narrow band-gap semiconductors and QED

We already learned that at a distance of a few source radii the potential drops to a value of the order $e\gamma^{-1/2}/\epsilon a$. This corresponds to the energy scale $e\varphi \simeq \Delta(Z_{xx}/Z)^{1/3}$, which is much larger than the energy gap Δ if the charge Z is significantly smaller than the characteristic charge

$$Z_{xx} \simeq \gamma^{-3/2} \simeq Z_x^3. \tag{65}$$

Then the analysis just given for WS will also be applicable in the NBGS/QED case with the conclusion that within several impurity radii the solution to the problem continues to be given by the MVP results, Eqs. (49)–(54), with $x \to r - a$.

The characteristic charge (65) separates the regime of moderately strong screening $\gamma^{-1/2} \ll Z \ll \gamma^{-3/2}$ to which the results of this subsection apply, from that of superstrong screening $Z \gg \gamma^{-3/2}$. The characteristic charge Z_{xx} significantly exceeds the crossover charge Z_x, Eq. (48), separating the regimes of weak and strong screening response. In NBGS with $\gamma = 10^{-3}$, we find $Z_{xx} \simeq 30^3$, which even by condensed matter standards is very large. In QED, we obtain $Z_{xx} \simeq 3000^3$. In view of unrealistically large value of Z_{xx}, the analysis of the regime of superstrong screening $Z \gg Z_{xx} \simeq \gamma^{-3/2}$ is not pursued here.

At distances exceeding several source radii, we need to look at the equation

$$\frac{dq}{d\ell} = -\frac{2g\alpha}{3\pi}\left(q^2 - \frac{2qr}{\Lambda}\right)^{3/2}, \quad \ell = \ln\frac{r}{a}, \tag{66}$$

which generalizes Eq. (60). Now the charge decreases faster with position than its WS counterpart; when the right-hand side vanishes, i.e., the edge of the electron shell $r = R_{sc}$ is reached, the charge acquires its observable value q_∞ [see Eq. (30)] and stops changing thereafter. The form of the solution can be approximately captured by the WS result (61) (that remains relevant at distances $r \ll R_{sc}$); the value of q_∞ at R_{sc} can be estimated with logarithmic accuracy by equating $e\varphi$ to Δ. This is equivalent to terminating the flow equation (60) at the scale

$$\ell_{sc} = \ln\frac{R_{sc}}{a} \gg 1 \tag{67}$$

and identifying $q(\ell_{sc}) = q_\infty$. Then the observable charge q_∞ will satisfy the equation

$$q_\infty^2 \approx \frac{3\pi}{4g\alpha\ln(q_\infty\Lambda/a)} \tag{68}$$

whose consequence is that for a fixed there exists a nearly universal lower limit on the observable charge q_∞. In the point source limit $a \to 0$, we find $q_\infty = 0$, i.e., there is a complete screening of the field of a point charge at an arbitrary distance from it. For a realistic extended source, the approximate solution for the charge is

$$q_\infty = Q_\infty\alpha \approx \sqrt{\frac{3\pi}{4g\alpha\ln(\Lambda/a(g\alpha)^{1/2})}} \to \sqrt{\frac{9\pi}{4g\alpha\ln(Z_{xx}/Z)}}, \tag{69}$$

where in the last step, we specified to the practically important case of $a \propto Z^{1/3}$. The size of the space charge region is then given by Eq. (30). The electric field at the edge of the space charge region can be estimated as

$$E_{sc} = \frac{eq_\infty}{\epsilon\alpha R_{sc}^2} \simeq \alpha^{1/2}E_Z. \tag{70}$$

The fact that the field at the shell edge (70) is much smaller than the Zener field demonstrates the sharpness of the edge.

The solution (69) is accurate provided $\ln(Z_{xx}/Z)^{1/3} \gg 1$. For NBGS with $Z \simeq 400$ (10-nm impurity region) and $\gamma = 10^{-3}$, we find $\ln(Z_{xx}/Z)^{1/3} \approx 1.5$. This is not really in the regime where Eq. (69) applies, but suffices to estimate the charge (ignoring the logarithmic factor) as $Q_\infty = q_\infty/\alpha \simeq \lambda^{-1/2} \approx 30$, and the size of the space charge region $R_{sc} \simeq 30$ nm. In QED, we find $Q_\infty \simeq 3000$.

As the bare charge Z continues to increase within the $\gamma^{-1/2} \ll Z \ll \gamma^{-3/2}$ range of moderately strong screening, the observable charge (69) and size of the space charge region R_{sc} remain nearly constant increasing very slowly with Z. The size of the source region $a \propto Z^{1/3}$ grows faster with Z than R_{sc}, at $Z \simeq Z_{xx}$ the two meet, and the result (69) ceases to be applicable.

To summarize, in NBGS and QED in the regime of moderately strong screening $Z_x \ll Z \ll Z_{xx}$ the expressions for the observable charge (69) and radius of the space charge region (30) are nearly universal. They are manifestations of the nearly-universal "zero charge" behavior (61) in the WS case. The physical mechanism by which the zero charge situation is avoided is purely classical: when it is no longer energetically favorable, the creation of further space charge terminates.

3. *Numerical solution*

To put our analysis of the regime of moderately strong screening $\gamma^{-1/2} \ll Z \ll \gamma^{-3/2}$ onto solid footing, we solved the full Eq. (38) numerically. The results are shown in Fig. 1, where we additionally displayed the charge $Q(r)$ within a sphere of radius r as an indicator of the strength of screening.

The very weak dependence of the observable charge $Q_\infty = q_\infty/\alpha$ and size R_{sc} of the space charge region on the bare charge Z has its origin in the Z dependence of the size of the source region (24). For $a =$ const, our theory predicts Z-independent limit on Q_∞ and R_{sc}. Therefore in order to single out this effect, we chose $a =$ const. Specifically, we set $Z_0 = \epsilon\Delta a/e^2 = 1$ (other values of Z_0 are equivalent to a rescaling $Z \to Z/Z_0$

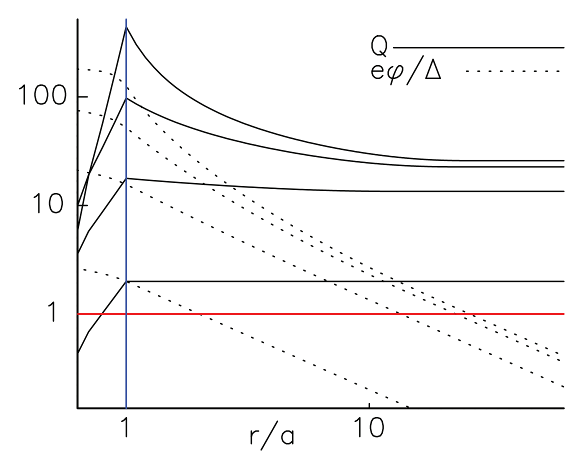

FIG. 1. (Color online) Potential φ (27) and charge $Q(r)$ within a sphere of radius r (57) as functions of distance (double logarithmic representation). The source region is $r/a < 1$. The gap value Δ is indicated by the horizontal line; the electron cloud is limited to the region where $e\varphi > \Delta$, which defines R_{sc}. The curves are drawn for $Z = 2,20,200,2000$, $\gamma = 0.001$. For large Z, R_{sc} approaches a Z-independent limit, indicating that $Q(r)$ tends to an upper bound Q_∞.

and $\gamma \to \gamma Z_0^2$). Several features of the numerical solution illustrating our analysis deserve mentioning. (i) As expected the screening effect of the space charge becomes noticeable for $\gamma Z^2 \gtrsim 1$. (ii) The crossing of the charge curves for $Z = 200$ and 2000 at r small is a direct illustration of screening: the TF screening length κ^{-1} [see Eq. (47) for $a = \text{const}$] is smaller for $Z = 2000$ than $Z = 200$, so that the screening at the central region is more complete in the former case. (iii) The large drop of the potential within a few radii of the impurity, clearly seen in the $Z = 200$ and $Z = 2000$ curves, is an illustration of our observation made in the analysis of the WS problem that within this range the potential must drop by a large factor of $(\gamma Z^2)^{1/6}$. (iv) Remarkably, for $Z \gg 1$ there exists a Z-independent limit on $R_{\rm sc}$ and Q_∞ whose values agree with our estimates.

VI. WEAK SCREENING REGIME $\lambda Z^2 \ll 1$ AND SYNTHESIS

The analysis carried out so far relied on the concept of the TF screening length κ^{-1}, Eq. (47), which in the weak-screening regime $\gamma Z^2 \ll 1$ loses its meaning as a length scale characterizing the source region, and one has to start anew. On the other hand, weak screening means that electron-electron interactions can (possibly) be treated by a perturbation theory. To lowest order in $\gamma \ll 1$, we set $\varphi = \varphi_{\rm ext}$, and then Eq. (33) gives

$$n(\mathbf{r}) = \frac{\gamma}{4\pi}\left[\frac{\epsilon\varphi_{\rm ext}(\mathbf{r})}{e}\left(\frac{\epsilon\varphi_{\rm ext}(\mathbf{r})}{e} - \frac{2}{R_e}\right)\right]^{3/2}. \tag{71}$$

For $r \leqslant a$, we have $\epsilon\varphi_{\rm ext}/e \simeq Z/a \simeq Z^{2/3}/R_e \gg 1/R_e$. Then the density of the space charge inside the source region can be estimated as $n \simeq \gamma Z^3/a^3$, implying that the number of electrons residing at $r \leqslant a$, is of the order γZ^3. The latter must be much smaller than the bare charge Z (to justify the approximation $\varphi = \varphi_{\rm ext}$) thus specifying the condition of weak screening as $\gamma Z^2 \ll 1$.

Outside of the impurity region, Eq. (71) becomes

$$n(r) = \frac{\gamma Z^3}{4\pi r^3}\left(1 - \frac{2r}{z\Lambda}\right)^{3/2}, \quad r \leqslant R_{\rm sc} = \frac{z\Lambda}{2}, \tag{72}$$

and $n = 0$ otherwise. The total screening charge is then of order $\gamma Z^3 \ll Z$, so that $q_\infty = z$ (or $Q_\infty = Z$), consistent with the TF relationship, Eq. (30). The electric field at the boundary of the space charge region can be estimated as

$$E(R_{\rm sc}) = \frac{q_\infty e}{\epsilon\alpha R_{\rm sc}^2} \simeq \frac{1}{z}E_Z, \tag{73}$$

which in view of the condition $z \gg 1$ demonstrates the sharpness of the boundary of the space charge region. Since the space charge residing at $r \leqslant a$ is small, Eq. (72) can be used to compute with logarithmic accuracy the net charge $q(r)$ within a sphere of radius $r > a$.

A. Weyl semimetal

In the WS case when $R_e = \infty$, the density of the space charge is given by

$$n(r) = \frac{\gamma Z^3}{4\pi r^3} = \frac{gz^3}{6\pi^2 r^3}, \tag{74}$$

and we find

$$q(r) \approx z - 4\pi\alpha\int_a^r y^2 n(y)dy = z\left(1 - \frac{2g\alpha z^2}{3\pi}\ln\frac{r}{a}\right). \tag{75}$$

This expression is applicable provided $(2g\alpha z^2/3\pi)\ln(r/a) \ll 1$, i.e., it inevitably fails at sufficiently large distance from the source.

Alternatively, the weak screening $\gamma Z^2 \ll 1$ analysis can be carried out by treating the cubic term of (58) perturbatively. Then the lowest-order solution outside the source is $\chi\alpha = z$. The next order gives for $r > a$,

$$\chi\alpha = z\left(1 - \frac{2g\alpha z^2}{3\pi}\ell\right) = z\left(1 - \frac{2g\alpha z^2}{3\pi}\ln\frac{r}{a}\right). \tag{76}$$

We observe that the expression for charge (57) (in natural units) computed with the help of Eq. (76) agrees with Eq. (75) to logarithmic accuracy which we adopt. Then the perturbative expression (76) may be regarded as a charge itself: it tells us that within the cloud, the physical potential φ and the density of space charge n decrease with r faster than $1/r$ and $1/r^3$, respectively.

On the other hand, no matter what the strength of screening is, at sufficiently large distances from the source center the charge $q(r)$ is given by the asymptotic limit of Eq. (61). All these results can be summarized in a simple interpolation formula for the charge $q = \chi\alpha$:

$$q^2(r) = \frac{z^2}{1 + (4g\alpha z^2/3\pi)\ln(r/a)}. \tag{77}$$

If the parameter z is viewed more broadly as the *net* charge within the source region, then this equation with $z = z^* \simeq \alpha^{-1/2}$ also covers the regime of strong screening $\gamma Z^2 \gg 1$ [see Eq. (61)]. This choice additionally guarantees that the results of Sec. V B2 pertinent to the NBGS/QED case are automatically captured.

Substituting $\chi = q/\alpha$ into Eqs. (56) and (33), we find corresponding interpolation formulas for the potential

$$\varphi(r) = \frac{Ze}{\epsilon r\sqrt{1 + (4g\alpha z^2/3\pi)\ln(r/a)}} \tag{78}$$

and the electron density

$$n(r) = \frac{gz^3}{6\pi^2 r^3[1 + (4g\alpha z^2/3\pi)\ln(r/a)]^{3/2}}. \tag{79}$$

The logarithmic terms in the denominators of Eqs. (77)–(79) are relevant at the scales r exceeding

$$R_{\rm scr} \simeq a e^{3\pi/4g\alpha z^2}. \tag{80}$$

This quantity is the screening length within the space charge of Weyl electrons. Deviations from the Coulomb law become substantial for $r > R_{\rm scr}$ and the asymptotic regimes of Eqs. (61)–(63) are reached at $r \gg R_{\rm scr}$. Specifically, as the strength of screening increases from small to large γZ^2, the screening radius (80) decreases from a very large value to the scale comparable to the source size.

Since the zero charge effect is an artifact, consistency of the theory requires that the screening length (80) to be significantly shorter than the radius of the electron cloud (64). Since $z \gg 1$, this is indeed true.

B. Narrow band-gap semiconductors and QED

The NBGS/QED case will be handled in exactly the same manner as that of the regime of moderately strong screening by terminating the WS solution at the scale of the space charge region (67). Then the observable charge follows from Eq. (77) as

$$q_\infty^2 \approx \frac{z^2}{1 + (4g\alpha z^2/3\pi)\ln(q_\infty \Lambda/a)}. \tag{81}$$

We see that the initial growth of $q_\infty(z)$ as z, in the regime of weak screening $\gamma Z^2 \simeq \alpha z^2 \ll 1$, slows down eventually saturating, in the strong screening regime $\gamma Z^2 \simeq \alpha z^2 \gg 1$, at z-independent value implied by Eq. (68). In the regime of weak screening, the solution to Eq. (81) one step beyond the zero-order $q_\infty \approx z[1 - (2g\alpha z^2/3\pi)\ln(z\Lambda/a)]$ reproduces previous findings.[6]

The dependence of the observable charge Q_∞ of a supercharged heavy nucleus on the bare charge Z was evaluated in Ref. 5 by numerically solving the TF theory discussed in our paper. The $Q_\infty(Z)$ dependence was found to be a monotonically increasing function with growth rate decreasing with Z; for $Z \to \infty$, the function $Q_\infty(Z)$ was found to grow slower than Z. The MVP theory[6] explained the $Q_\infty(Z)$ behavior in the regime of weak screening $\gamma Z^2 \ll 1$ and laid out a foundation to understand the regime of strong screening $\gamma Z^2 \gg 1$; its place in the problem of screening of overcritical external charge was explained earlier. However, the zero-charge-type solution of the TF theory in the WS case was missed whose consequences are the following: (i) for a fixed, the observable charge Q_∞ saturates as $Z \to \infty$ at a Z-independent value and, (ii) for realistic $a \propto Z^{1/3}$, the $Q_\infty(Z)$ dependence is a nearly universal slowly increasing function of Z, see Eq. (69), which goes beyond explanation of numerical results.[5]

VII. DEFICIENCIES AND IMPROVEMENT OF THE THOMAS-FERMI THEORY

Even though in the NBGS/QED case complete screening does not occur, there are other respects in which the TF theory is internally inconsistent. Solving Eq. (81) for the bare charge z, we find

$$z^2 \approx \frac{q_\infty^2}{1 - \left(4g\alpha q_\infty^2/3\pi\right)\ln(q_\infty \Lambda/a)}. \tag{82}$$

While correctly predicting that the latter is always larger than the observable charge, Eq. (82) also tells us that for fixed q_∞ and $a \to 0$ the denominator vanishes for finite a given by

$$a_p \simeq \Lambda q_\infty e^{-3\pi/4g\alpha q_\infty^2} \tag{83}$$

before the limit of point source is reached. At $a = a_p$, the bare charge is infinite, while for $a < a_p$, it is imaginary; the latter feature is certainly unacceptable. These conclusions having their origin in the "zero charge" solution in the WS case, like the zero charge effect itself, are artifacts. Even if the vanishing of the observable charge did occur, the scale (83) is too small to be of any practical importance.

In Sec. IV A, we introduced a modified TF equation (41) with built-in quantum-mechanical fall to the center. It is straightforward to realize that such a modification removes the zero charge effect in the WS case; the NBGS/QED problems are also liberated of the difficulty of the vanishing denominator. Specifically, in the WS ($\Delta = 0$) case, substituting (56) into (41), we obtain [instead of (60)] the following flow equation:

$$\frac{dq}{d\ell} = -\frac{2g\alpha}{3\pi}(q^2 - 1)^{3/2}. \tag{84}$$

Now any "initial" charge $q(0) = z > 1$ will be carried to the stable fixed point $q = 1$, which is reached as $\ell \to \infty$. Equation (84) can be integrated in quadratures for arbitrary initial z with the result

$$q^2(\ell) - 1 = \frac{1}{(2g\alpha/3\pi)^2(\ell + \ell_W)^2 - 1}, \tag{85}$$

where the scale $\ell_W = 3\pi z/(2g\alpha\sqrt{z^2-1})$ is determined by the condition $q(\ell = 0) = z$. The corresponding spatial scale

$$R_W = a e^{\ell_W} = a \exp\left(\frac{3\pi}{2g\alpha}\frac{z}{\sqrt{z^2 - 1}}\right) \tag{86}$$

characterizes the size of the space charge cloud. For $r \gg R_W$, the (overcritical) impurity charge appears as being poised at the critical value. As $z \to 1 + 0$ (a weakly overcritical source), the cloud size (86) diverges because the creation of spacial charge is a critical phenomenon. The Kosterlitz-Thouless-type essential singularity in (86) is typical of localization transitions related to the quantum-mechanical fall to the center.[22] For the supercritical source $z \gg 1$, the cloud size becomes Eq. (64). The point source limit $a \to 0$ ($\ell = \infty$) of the solution (85) also describes the NBGS/QED problems with the conclusion that at arbitrary distance r from an overcritical point source the observable charge of the latter is unity.

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