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High-energy wave functions for the screened Coulomb field*

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An eikonal formalism is developed to calculate corrections due to screening to the exactly solvable case of the unscreened Coulomb field. The high-energy Sommerfeld-Maue wave functions are used, and, by construction, the unscreened case is reproduced exactly for all coordinate space. The modification caused by screening is found to be multiplicative, and it appears as a phase factor $\exp\{\mp iZe^2(E/p)\ln[p(r\pm z)] - i(E/p) \times \int_{\pm\infty}^{z} V(\rho,\xi)\,d\xi\}$, where p is a large momentum, E is the corresponding relativistic energy, and V is the screened Coulomb field. Our approximate high-energy wave function is given by one formula for all coordinate values, without any need to introduce partial waves, is easy to calculate numerically, and is shown to satisfy a second-order differential equation to a very good accuracy practically in the whole space. For example, the outgoing solution satisfies an appropriate equation to an accuracy better then 3% in a very large region of cylindrical variables $\rho \geq 0.1$, $z \leq 2p$, which expands with increasing p.

I. INTRODUCTION

The routine way to evaluate wave functions for a given spherically symmetric potential is to use the partial-wave expansion. However, for large energies, and especially for particles with spin, the number of partial-wave amplitudes is so big that it becomes essentially a numerical problem to include sufficiently many of them. For a special case of the unscreened Coulomb field, using the high-energy Sommerfeld-Maue approximation, one can analytically sum up all partial-wave amplitudes and get a compact form for the whole wave function. But, to account for screening, often given only numerically, one must use an approximate scheme.

The aim of our paper is to propose such an approximation which completely bypasses the partial-wave expansion, is as close as possible to the known exact solution, and by one formula valid practically in the whole space, describes the deviations from the known solution of the unscreened case. The motivation of our work is the application of our wave functions for the evaluation of the high-energy bremsstrahlung, pair production, and elastic scattering in the presence of a given screened Coulomb field. The relativistic, quantum theory of these processes was fully developed many years ago by Bethe and Maximon,[1] and extended by Olsen, Maximon, and Wergeland.[2] For all details, in particular on the high-energy Sommerfeld-Maue wave functions, we refer to these papers. Here we only mention, that these wave functions are approximate solutions of the iterated Dirac equation and are given by

$$\psi = \exp(i\vec{p}\cdot\vec{r})(1-\tfrac{1}{2}i\vec{\alpha}\cdot\vec{\nabla}/E)F^{\text{in,out}}u, \tag{1.1}$$

where $\vec{\alpha}$ and u are Dirac matrices and a Dirac spinor, respectively, E is the relativistic energy (in units where $m=c=\hbar=1$) given by $E=(p^2+1)^{1/2}$, p is a large momentum, and $F^{\text{in,out}}$ are the appropriate solutions of the equation

$$(\nabla^2 + 2i\vec{p}\cdot\vec{\nabla} - 2EV)F = 0. \tag{1.2}$$

It is known that for the special case of the unscreened Coulomb potential

$$V = V_c \equiv -Ze^2 r^{-1},$$

the exact solution of Eq. (1.2) is given in a compact form in terms of the confluent hypergeometric function as

$$F_c^{\text{in,out}} = \Gamma(1 \pm iZe^2E/p)\exp(\tfrac{1}{2}\pi Ze^2E/p) \times {}_1F_1(\mp iZe^2E/p; 1; \mp ipr - i\vec{p}\cdot\vec{r}). \tag{1.3}$$

Equations (1.2) and (1.3) are the starting points of our considerations. In this paper we always have in mind the Sommerfeld-Maue wave functions. However, our method is more general and can be applied if two conditions are satisfied: (a) there is a known exact solution for a special case, and (b) there is a "large" parameter in the problem. For example, in the field of heavy-ion reactions the large parameter is the ratio of the distance of closest approach to the Compton wavelength, while the exact solution corresponds to the Coulomb potential and the square well. Details of this application shall be given in another paper.

Staying with the Sommerfeld-Maue wave functions, we call Eq. (1.2) the exact equation. This equation we replace in Sec. II by a first-order differential equation. By construction, the last equation has to have the exact F_c, given by Eq. (1.3), as its solution for the special case $V=V_c$. For V which differs from V_c at large distances, but is very close to V_c at small distances, we find the solution in a form F_c times a correcting phase factor. A special care of the boundary conditions enables us to remove the logarithmic phase factor out of F_c.

To justify our result we estimate in Sec. III the errors which appear when our solution is put into the exact second-order differential equation. In this way we can locally check at each point in configuration space the goodness of our solution and find out the accuracy with which the exact second-order differential equation is satisfied. We provide an upper bound for this accuracy.

As an illustration of our result we calculate numerically in Sec. IV the contours of a constant correcting phase. Looking at the number of such contours in a given region of configuration space, we can see the effect of screening as the modification of the unscreened solution F_c. This effect is studied as a function of the charge of a nucleus and momentum of electron (position).

Our result must be compared with the one obtained many years ago by Olsen, Maximon, and Wergeland (OMW).[2] On the level of the F function we make the following remarks. OMW use two different techniques in different regions of configuration space, while we have one method covering both regions. We never need to go through the partial-wave expansion, while OMW have to use it in one region of space. OMW use WKB-type methods to evaluate the whole result, while in our case the eikonal method is used only for the evaluation of a correcting factor, multiplying F_c. For the special case $V=V_c$ our result, by definition, agrees with the exact one in the entire configuration space, while OMW in one region of space have the agreement with the small-angle approximation of the exact result, and in another region of space they have to take special care to avoid divergence and to get the proper logarithmic phase factor. For the screened potential $V\neq V_c$ in the region where both cylindrical variables ρ and z are large, the result of OMW is close to ours. It is so, because to reach this region along a path parallel to the z axis one meets either the small V, or the small $V_1=V-V_c$. However, to reach another region of space, namely, $\rho\approx 1$ and $|z|\approx p$, one has to pass through the region $\rho\approx 1$ and very small z. Then, one cannot work with the first-order differential equation in which V is in the inhomogeneous term, because the variation of V is comparable with V itself. One is then forced to change the method as OMW did. On the other hand, if one is calculating only the correction to F_c, and has V_1 instead of V, one can use the first-order differential equation since the large variation of F is in F_c, while the correcting phase is very mildly varying along the whole path.

Finally, our result for F stated as

$$F=F_c\times(\text{eikonal correction}),$$

may be associated with a similar result obtained in a different field, namely, the large-angle pp scattering, discussed by Gaisser.[3] There, the soft exchanges, worked out in the eikonal framework elaborated by Erickson, Fried, and Gaisser,[4-6] are modifying the hard exchange, which takes care of the large scattering angle. Our F_c, although not the first Born term but the whole solution for $V=V_c$, plays a similar role as the hard exchange does, and enables us to reach practically all points in configuration space.

II. FIRST-ORDER DIFFERENTIAL EQUATION

For a given screened potential V we want to replace the exact second-order differential equation (1.2) by a simply solvable first-order differential equation. There are many ways of achieving this, and our choice is specified by the following two requirements: (i) The exact solution (1.3) of the exact second-order equation (1.2) has to be also the exact solution of our first-order equation for $V=V_c$ in the whole configuration space. (ii) The basic part of the first-order differential operator is the simplest one, already appearing in the exact equation (1.2). It is $2i\vec{p}\cdot\vec{\nabla}$. We choose the z axis along the incoming (outgoing) momentum $\vec{p}$, and denote cylindrical coordinates perpendicular to $\vec{p}$ by $\vec{\rho}$, having $2i\vec{p}\cdot\vec{\nabla}=2ip\,\partial/\partial_z$ and $r^2=\rho^2+z^2$.

Both of our requirements are satisfied if we take the following first-order differential equation:

$$[2ip\,\partial/\partial_z+A(\vec{\rho},z)-2EV_c]F_c=0, \tag{2.1}$$

where F_c is given by Eq. (1.3), and the new function $A(\vec{\rho},z)$ by definition, has to guarantee the equality in Eq. (2.1). The explicit form of $A(\vec{\rho},z)$ is unimportant for us, since we are only interested in the solution of our first-order differential equation, which in the case $V=V_c$ is already known. The implicit definition of $A(\vec{\rho},z)$ can be given by writing the solution of Eq. (2.1) as

$$F_c(\rho,z)=B\exp\left(-i\frac{E}{p}\int_{z_0(\rho)}^{z}[V_c(\rho,\xi)-\tfrac{1}{2}E^{-1}A(\vec{\rho},\xi)]\,d\xi\right), \tag{2.2}$$

where B is independent of z, and $z_0(\rho)$ shall be determined from the boundary conditions in the following paragraph.

We now pass on to the screened potential V, which we split up into two parts,

$$V=V_c+V_1, \tag{2.3}$$

where V_1 is a small and smooth potential, as explicitly shown in Appendix B, contrary to both V and V_c, which at small distances are big and strongly varying. As the most obvious generalization of Eq. (2.1) we postulate for $V=V_c+V_1$ the similar first-order differential equation for F as Eq. (2.1) for F_c. Thus, we write

$$\left(2ip\frac{\partial}{\partial z}+A(\vec{\rho},z)-2E(V_c+V_1)\right)F=0, \tag{2.4}$$

and verify in Sec. III that, for large p, the solution of Eq. (2.4) satisfies to a very good accuracy the exact equation (1.2) for F, practically in all of configuration space.

The solution of Eq. (2.4) is simply given by

$$F=F_c\exp\left(-i\frac{E}{p}\int_{z_0(\rho)}^{z}V_1(\rho,\xi)d\xi\right), \tag{2.5}$$

and it should be reemphasized, that the explicit form of the function $A(\vec{\rho},z)$ is unimportant, since it is hidden in the known function F_c. To specify $z_0(\rho)$ we have to consider the boundary conditions. For definiteness let us take the outgoing solution. It is well known that for $z\to-\infty$ the exact solution F_c^{out} of the exact Eq. (1.2) for the unscreened $V=V_c$ behaves as

$$F_c^{\text{out}} \underset{z\to-\infty}{\simeq} \exp\{-iZe^2(E/p)\ln[p(r-z)]\}. \tag{2.6}$$

On the other hand, the corresponding exact solution of the exact equation (1.2) for the screened potential $V\neq V_c$ has to be such that the product

$$[\exp(ipz)]F^{\text{out}}$$

behaves as a plane wave for $z\to-\infty$, because of the finite range of the screened V. These two statements on the exact boundary conditions we want to fully respect. Therefore, we demand that in our solution, given by Eq. (2.5), there is a compensation effect and the logarithmic phase factor of F_c is cancelled by an appropriate phase factor of the second part of the right-hand side of Eq. (2.5). This requirement determines for us $z_0(\rho)$, and we can write the condition for $z_0(\rho)$ either in the form containing V_1 as

$$\int_{z_0(\rho)}^{z}V_1(\rho,\xi)\,d\xi \underset{z\to-\infty}{\simeq} -Ze^2\ln[p(r-z)], \tag{2.7a}$$

or in the form containing V and $z=-\infty$ as

$$\int_{-\infty}^{z_0(\rho)}V(\rho,\xi)\,d\xi=Ze^2\ln[\rho^2p/(z_0+r_0)], \tag{2.7b}$$

where $r_0^2\equiv\rho^2+z_0^2$ and $\rho^2=(r-z)(r+z)$.

Both Eqs. (2.7a) and (2.7b) define $z_0(\rho)$, but in a rather involved way. Luckily enough we do not have to find explicitly $z_0(\rho)$, but using Eqs. (2.7b) and (2.5) we can eliminate $z_0(\rho)$ altogether and write our solution of Eq. (2.4) in terms of V instead of V_1. We get

$$F^{\text{out}}=F_c^{\text{out}}\exp\left(iZe^2(E/p)\ln[p(r-z)] -i(E/p)\int_{-\infty}^{z}V(\rho,\xi)\,d\xi\right). \tag{2.8a}$$

Similarly, for the incoming solution we find

$$F^{\text{in}}=F_c^{\text{in}}\exp\left(-iZe^2(E/p)\ln[p(r+z)] +i(E/p)\int_{z}^{\infty}V(\rho,\xi)\,d\xi\right). \tag{2.8b}$$

Our final result, written in Eqs. (2.8a) and (2.8b) is stated in the most practical form for any given screened potential V. However, to study the limiting case $V=V_c$ one has to reintroduce again $z_0(\rho)$ to avoid divergence, and then the form of our solution given in Eq. (2.5) is easier to deal with.

The solution of our Eq. (2.4), stated either in Eq. (2.5), or in Eqs. (2.8a) and (2.8b), can be shortly written as

$$F=F_c\exp(i\chi). \tag{2.9}$$

The correcting phase χ, which takes care of screening, satisfies the first-order differential equation

$$\frac{\partial}{\partial z}\chi=-\frac{E}{p}V_1, \tag{2.10}$$

which follows directly from Eqs. (2.9), (2.4) and (2.1). The important feature of Eq. (2.10), besides its simplicity, is, that its inhomogeneous term is small and smooth in the whole configuration space. This is illustrated in an example in Appendix B.

III. ESTIMATES OF ERROR

To justify our result we return to the exact equation (1.2) for F, and consider the screened potential $V\neq V_c$. We look for the solution of Eq. (1.2) in the form

$$F=F_c\exp(i\chi), \tag{3.1}$$

being guided by the result of Sec. II. However, contrary to Sec. II, we now consider the second-order differential equation both for F_c and χ. According to Eqs. (1.2) and (3.1), F_c and χ satisfy the following equations

$$(\nabla^2+2i\vec{p}\cdot\vec{\nabla}-2EV_c)F_c=0, \tag{3.2}$$

$$\tfrac{1}{2}p^{-1}[i\nabla^2\chi-(\vec{\nabla}\chi)^2]+\left(\frac{i}{p}\frac{\vec{\nabla}F_c}{F_c}-\frac{\vec{p}}{p}\right)\cdot\vec{\nabla}\chi=\frac{E}{p}V_1. \tag{3.3}$$

The boundary conditions for χ are just the one given in Sec. II. For example, the outgoing solution has to fulfill

$$\chi(\rho,z) \underset{z\to-\infty}{\simeq} Ze^2(E/p)\ln[p(r-z)]. \tag{3.4}$$

It is useful to split up the χ introduced in Eq. (3.1) into a sum $\chi_0+\chi_1$ in such a way that, by definition, χ_0 satisfies the first-order differential equation

$$\vec{a}\cdot\vec{\nabla}\chi_0=(E/p)V_1, \tag{3.5}$$

where

$$\vec{a} \equiv \frac{i}{p}\frac{\vec{\nabla}F_c}{F_c} - \frac{\vec{p}}{p},$$

and χ_0 obeys the full boundary condition, given by Eq. (3.4). The remaining part of χ has to fulfill the zeroth boundary condition, and satisfy the equation

$$\begin{aligned} &\tfrac{1}{2}p^{-1}[i\nabla^2\chi_1 - (\vec{\nabla}\chi_1)^2 - 2(\vec{\nabla}\chi_0)\cdot(\vec{\nabla}\chi_1)] \\ &+\vec{a}\cdot\vec{\nabla}\chi_1 = \tfrac{1}{2}p^{-1}[-i\nabla^2\chi_0 + (\vec{\nabla}\chi_0)^2]. \end{aligned} \tag{3.6}$$

Equations (3.5) and (3.6) are meaningful at all points for which $F_c \neq 0$.[7]

The term $\vec{\nabla}F_c/F_c$ is studied in detail in Appendix A, where dimensionless quantities p^{-1}, 1, and p are used to define regions of configuration space and orders of magnitude. We find that excluding a very small region

$$\rho, |z| \lesssim p^{-1}, \tag{3.7}$$

$|\vec{\nabla}F_c/F_c|$ behaves at most as 1. Therefore, cutting out from our consideration a strip

$$\rho \lesssim p^{-1}, \quad z \gtrsim -p^{-1} \tag{3.8}$$

for the outgoing solution, and a strip

$$\rho \lesssim p^{-1}, \quad z \lesssim p^{-1}$$

for the incoming solution, we can approximate

$$\vec{a} \approx -\vec{p}/p,$$

and take all results from Sec. II as the results for χ_0.[8]

Having explicit form of χ_0, we can investigate the inhomogeneous term in Eq. (3.6) for χ_1. The modulus of this term is bounded by

$$\tfrac{1}{2}p^{-1}\left(\left|\frac{\partial^2\chi_0}{\partial\rho^2}\right| + \left|\rho^{-1}\frac{\partial\chi_0}{\partial\rho}\right| + \left|\frac{\partial^2\chi_0}{\partial z^2}\right| + \left|\frac{\partial\chi_0}{\partial\rho}\right|^2 + \left|\frac{\partial\chi_0}{\partial z}\right|^2\right). \tag{3.9}$$

Individual derivatives of χ_0 are estimated in Appendix B. There, we restricted ρ from below even more than in Eq. (3.8), setting

$$\rho \gtrsim 0.1. \tag{3.10}$$

However, this restriction is harmless, from the point of view of applications, since there the lowest interesting value of ρ is around 1. Taking the estimates from Eqs. (B4), (B6), (B7), and (B9), and using Eq. (3.9), we get

$$\tfrac{1}{2}p^{-1}|-i\nabla^2\chi_0 + (\vec{\nabla}\chi_0)^2| < 8p^{-1}\lambda^2 \approx 1.1p^{-1}10^{-2}, \tag{3.11}$$

where $\lambda = 2(\frac{3}{4}\pi)^{-2/3}e^2Z^{1/3}$, and $\lambda = 0.038$ for $Z = 100$. It is indeed a very small quantity for large p, and remembering that χ_1 has to fulfill the zeroth boundary condition, it is plausible, though not proven because of the nonlinearity of equation, that χ_1 is varying very slowly.

We expect that the phase χ can be very well approximated by χ_0 in a bounded region of space, where the constant phase is immaterial. To verify that $\chi \approx \chi_0$ satisfies approximately Eq. (3.3), we compare Eqs. (3.3) and (3.5), and find the accuracy to which the omitted terms are neglected with respect to the remained one. In this way we can check locally at every point of space to what accuracy the known function χ_0 is the solution of the second-order differential equation (3.3). It should be remembered that our whole solution for F is $F_c\exp(i\chi_0)$ and F_c satisfies *exactly* Eq. (3.2). Let us denote the accuracy connected with χ_0 by d, and write down the expression for it according to the above definition

$$d = \frac{\frac{1}{2}p^{-1}|i\nabla^2\chi_0 - (\vec{\nabla}\chi_0)^2|}{(E/p)V_1}. \tag{3.12}$$

The numerator is already estimated in Eq. (3.11), while the denominator is a decreasing function of r, behaving as $0.73/r$ for large r, if $Z = 100$. For $r \lesssim \xi p$, where ξ is a given number, we get from Eqs. (3.11) and (3.12)

$$d \lesssim 1.5\xi 10^{-2}. \tag{3.13}$$

Thus, if we take $r \lesssim 2p$, we get $d \lesssim 3\%$.

The estimates of partial derivatives of χ_0 with respect to z and ρ, given in Eqs. (B4)–(B9), are too pessimistic in some regions of configuration space. In particular, considering the outgoing solution and large negative z, we have from our asymptotic condition Eq. (3.4) that

$$\chi_0 \underset{z\to-\infty}{\sim} 0.73\ln[p(r+|z|)], \tag{3.14}$$

$$\begin{aligned} &\left|\frac{\partial\chi_0}{\partial z}\right| < |z|^{-1}, \quad \left|\frac{\partial^2\chi_0}{\partial z^2}\right| < |z|^{-2}, \\ &\left|\frac{\partial\chi_0}{\partial\rho}\right| < |z|^{-1}, \quad \left|\rho^{-1}\frac{\partial\chi_0}{\partial\rho}\right| \approx \left|\frac{\partial^2\chi_0}{\partial\rho^2}\right| < |z|^{-2}. \end{aligned} \tag{3.15}$$

For very large $|z| = -z$, and fixed ρ we have $V_1 \approx |z|^{-1}$, and the accuracy d, defined in Eq. (3.12), is

$$d \leq 2.5p^{-1}|z|^{-1}. \tag{3.16}$$

Therefore, taking for example $|z| = 2p$, we get a very good accuracy for large p. This result is not surprising, because for the outgoing solution we are bound to get a very good approximation for large negative z, since we obeyed the exact boundary condition at $-\infty$. Similarly, for the incoming solution we get a very good accuracy in satisfying Eq. (3.3) for large positive z.

Another region of configuration space where the bounds given in Eqs. (B4), (B6), (B7), and (B9) are too pessimistic is the region of large ρ, for example, $\rho \approx p$, and arbitrary z. There, using Eqs. (B4) and (B9), we get

$$\left|\frac{\partial \chi_0}{\partial \rho}\right| < 1.5\rho^{-1}, \quad \left|\rho^{-1}\frac{\partial \chi_0}{\partial \rho}\right| < 1.5\rho^{-2}, \quad \left|\frac{\partial^2 \chi_0}{\partial \rho^2}\right| < 1.5\rho^{-2}. \tag{3.17}$$

For large $\rho > \lambda^{-1}$ and $|z| \lesssim \rho$ the potential V_1 behaves as ρ^{-1}, and the derivatives of χ_0 with respect to z are bounded by

$$\left|\frac{\partial \chi_0}{\partial z}\right| < \rho^{-1}, \quad \left|\frac{\partial^2 \chi_0}{\partial z^2}\right| < \rho^{-2}.$$

Thus, for large ρ the accuracy d, defined in Eq. (3.12), is

$$d \leqslant 3.7p^{-1}\rho^{-2}. \tag{3.18}$$

In particular for $\rho \approx p$, and large p we satisfy Eq. (3.3) with a very good accuracy for arbitrary $z \leqslant \rho$.

Including all results, stated in Eqs. (3.13), (3.16), and (3.18), we can say that for the outgoing solution we satisfy Eq. (3.3) to an accuracy better than 3% in a very large domain

$$\rho \geqslant 0.1, \quad z \leqslant 2p, \tag{3.19}$$

which expands with the increasing p. Our region (3.19) covers both regions $\rho \approx 1$, $|z| \approx p$, and $\rho \approx |z| \approx p$ interesting for bremsstrahlung and pair production.

IV. CONSTANT χ CONTOURS

To appreciate the importance of the correcting phase factor $e^{i\chi}$, and to get some feeling of it in different regions of configuration space, we plot contours of constant χ on the plane of cylindrical variables ρ and z. The number of such contours in a given region of space indicates how much we have to change F_c to account for screening. The change of χ by about 3 reverses the sign of F_c, while by 1.5 interchanges the real and imaginary parts of F_c. Thus, the number of contours of equal χ indicates the importance of screening and shows the necessity of including $e^{i\chi}$ together with F_c.

As an example of the screened potential V, we take the modified Thomas-Fermi potential[9,10]

$$V(r) = -Ze^2r^{-1}[0.711\exp(-0.175\lambda r) + 0.2889\exp(-1.6625\lambda r)]^2, \tag{4.1}$$

with $\lambda \equiv 2(\frac{3}{4}\pi)^{-2/3}e^2Z^{1/3}$. For the numerical evaluation of $\chi(\rho, z)$ we take the outgoing solution, written in the form

$$\chi(\rho, z) = Ze^2(E/p)\ln\{p[(\rho^2+z^2)^{1/2} - z]\} - (E/p)\int_{-\infty}^{z} V(\rho^2+\xi^2)^{1/2}d\xi$$

and evaluate it for two values of Z, 10 and 100, and two values of ρ, 100 and 500, in our dimensionless units $m=1$.

The following features of constant χ contours can be noted:

(i) Fixed p and Z, e.g., $p=100$, $Z=100$, (Fig. 1): (a) Going from left to right contours become flatter. However, the density of contours, measured parallel to the z axis, increases to a finite value if we approach the ρ axis from either left or right. This is in agreement with the decreasing behavior of V_1 for increasing r. Going parallel to the ρ axis towards small values of ρ we meet more contours, and their density is also finite. (b) Considering four regions: $\rho \approx 1, z \approx -p$; $\rho \approx 1$, $z \approx p$; $\rho \approx p, z \approx -p$; and $\rho \approx p, z \approx p$, most important for bremsstrahlung and pair production, the number of contours of equal χ is small and comparable in the first three regions and much bigger in the fourth region. It means that F_c is only slightly corrected by $e^{i\chi}$ in the first three regions and must be corrected in the fourth, where the effect of screening is the biggest.

(ii) Fixed p, varying Z, e.g., $p=100$, $Z=10$ 100 Figs. 1 and 2: (a) The main dependence of χ on Z is in $V_1 \sim Z$. Therefore, changing ten times Z we get a corresponding effect in χ. For this reason there are introduced broken-line contours in Fig. 2, corresponding to a change ten times smaller in χ than on the continuous contours. (b) The smaller number of contours in Fig. 2, compared to Fig. 1 in all four regions important for bremsstrahlung and pair production, indicates that F_c is a quite good approximation of F for low Z, and verifies the known fact that the im-

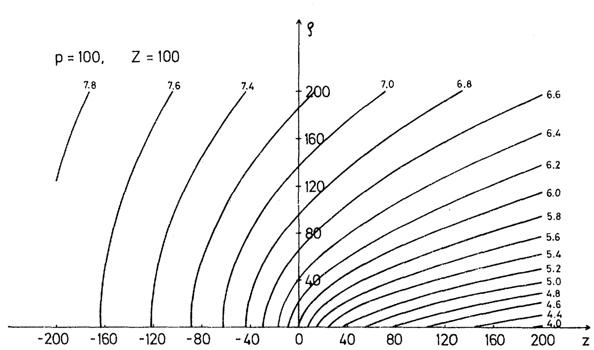

FIG. 1. Contours of constant correcting phase for the modified Thomas-Fermi potential; $p=100$ in units $m=1$, $Z=100$. The neighboring contours differ in phase by 0.2.

portance of screening increases with Z.

(iii) Varying p, fixed Z, e.g., $p=100, 500$, $Z=100$, (Figs. 1 and 3): (a) χ varies very slowly with p, with the main dependence given as an additive term $\ln p$. Therefore, contours in Figs. 1 and 3 are very much the same, though because of a different scale we have drawn contours separated by a different distance. (b) The derivatives of χ are practically independent of p, and the effect of flattening of contours of constant χ for large positive z is transparent in Fig. 3, which can be considered as an extension of Fig. 1.

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APPENDIX A. THE ESTIMATE OF $|\nabla F_c/F_c|$

Let us denote "of order p^{-1} or lower orders" as $\ll 1$, "of order p or higher orders" as $\gg 1$, and divide the configuration space of cylindrical variables (ρ, z) into the following four regions:

(1) $\rho \ll 1, \quad |z| \ll 1$,

(2) $\rho \ll 1, \quad 1 \lesssim |z|$, and $\rho \approx 1, \quad 1 \ll |z|$,

(3) $\rho \approx 1, \quad |z| \ll 1$, and $\rho \approx 1, \quad |z| \approx 1$,

(4) $1 \ll \rho$, z arbitrary.

We estimate $|\vec{\nabla} F_c/F_c|$ in each of these regions separately.

Region 1: $\rho \ll 1$, $|z| \ll 1$

Denote the argument of F_c as

$$u \equiv ip(r-z),$$

and note that in this region it is of order 1, or smaller, so we write

$$|u| \lesssim 1.$$

For such argument the function $F_c = \Gamma(1-in)e^{\pi n/2} \times {}_1F_1(in; 1; u)$, and its derivative with respect to u, denoted as F_c, behave so that

$$|F'_c/F_c| \approx 1, \quad \text{with } n = Ep^{-1}Ze^2.$$

The partial derivatives of u with respect to either z or ρ behave as

$$\left|\frac{\partial u}{\partial z}\right| = p|z(\rho^2+z^2)^{-1/2}-1| \lesssim p,$$

$$\left|\frac{\partial u}{\partial \rho}\right| = p\rho(\rho^2+z^2)^{-1/2} \lesssim p.$$

Therefore, we get

$$|\vec{\nabla} F_c/F_c| \lesssim p.$$

Region 2: $\rho \ll 1$, $1 \lesssim |z|$ and $\rho \approx 1$, $1 \ll |z|$

Here, we always have $\rho \ll |z|$, i.e., $\rho\, |z|^{-1} \ll 1$, or $\rho |z|^{-1} \lesssim p^{-1}$. Therefore, for positive $z > 0$ we get

$$u = ip|z|\left[(1+\rho^2|z|^{-2})^{1/2}-1\right]$$
$$\approx \tfrac{1}{2} ip\rho^2|z|^{-1},$$

from which it follows

$$|u| \lesssim 1, \quad |F'_c/F_c| \approx 1,$$

$$\left|\frac{\partial u}{\partial z}\right| \approx p\rho^2|z|^{-2} \lesssim p^{-1}, \quad \left|\frac{\partial u}{\partial \rho}\right| \approx p\rho|z|^{-1} \lesssim 1,$$

$$|\vec{\nabla} F_c/F_c| \lesssim 1.$$

For negative $z < 0$ we get

$$u = ip|z|\left[(1+\rho^2|z|^{-2})^{1/2}+1\right] \approx 2ip|z|,$$

and therefore the argument of F_c has a very large modulus. To estimate $|F_c|$ and $|F'_c|$ we use the

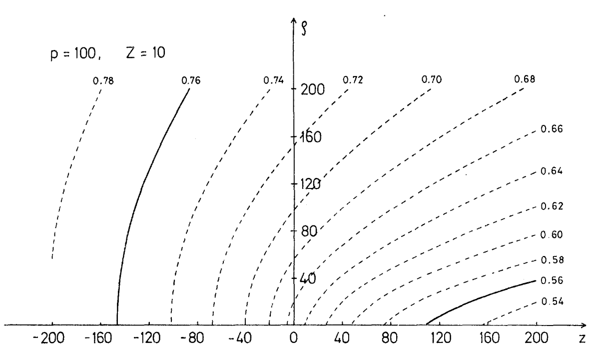

FIG. 2. Contours as in Fig. 1; $p=100$, $Z=10$. Broken lines are contours corresponding to phases differing by 0.02. Continuous lines are as in Fig. 1 and differ in phase by 0.2.

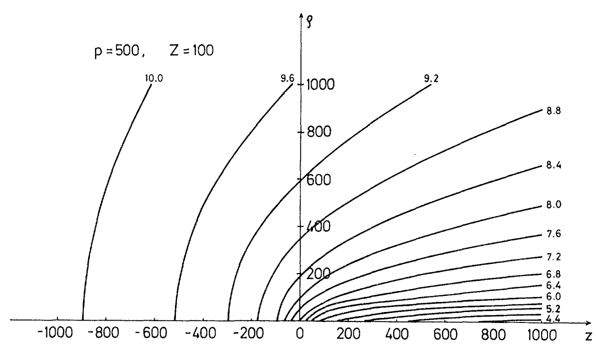

FIG. 3. Contours as in Fig. 1; $p=500$, $Z=100$. The neighboring contours correspond to phases differing by 0.4.

asymptotic expansion for ${}_1F_1$. Denoting $n \equiv Ep^{-1}Ze^2$, we have

$$F_c = \Gamma(1-in)\,e^{\pi n/2}\,{}_1F_1(in;1;u)$$
$$= \Gamma(1-in)[\Gamma(1-in)]^{-1}(-u)^{-in}g(in;in;-u)e^{\pi n/2}$$
$$+\Gamma(1-in)[\Gamma(in)]^{-1}(e^{u\pi n/2})u^{in-1}g(1-in;1-in;u), \tag{A1}$$

where

$$g(\alpha;\beta;u) \underset{(u)\to\infty}{\sim} 1+\alpha\beta/u+\cdots.$$

Therefore, we get

$$|F_c'/F_c| \approx |u|^{-1}. \tag{A2}$$

The partial derivatives of u behave as

$$\left|\frac{\partial u}{\partial z}\right| \approx p, \quad \left|\frac{\partial u}{\partial \rho}\right| \approx p\rho|z|^{-1} \lesssim 1.$$

Taking into account Eq. (A2), we get

$$|\vec{\nabla}F_c/F_c| \lesssim 1,$$

similarly as for the positive $z>0$.

Region 3: $\rho\approx 1, |z|\ll 1$ and $\rho\approx 1, |z|\approx 1$

Here $|u|\approx p$, so we apply the asymptotic expansion given in Eq. (A1), and get Eq. (A2). The partial derivatives $|\partial u/\partial z|$ and $|\partial u/\partial\rho|$ are of order ρ, so we get

$$|\vec{\nabla}F_c/F_c| \approx 1.$$

Region 4: $1\ll\rho$, z arbitrary

For $z<0$ we have $|u|\gtrsim p^2$, thus $|F_c'/F_c|\lesssim p^{-2}$. The partial derivatives of u behave as

$$\left|\frac{\partial u}{\partial z}\right| \approx p, \quad \left|\frac{\partial u}{\partial \rho}\right| \lesssim p.$$

Therefore

$$|\vec{\nabla}F_c/F_c| \lesssim p^{-1}.$$

For $z>0$, $|u| = p|(\rho^2+z^2)^{1/2}-z|$ may take any positive value. It is useful to consider separately three cases: $|u|\lesssim 1$, $|u|\approx p$, and $|u|\gtrsim p^2$. In the first case we must have $|z|\gtrsim p\rho^2$ and $|u|\approx \frac{1}{2}p\rho^2|z|^{-1}$. Thus,

$$|F_c'/F_c| \approx 1,$$
$$\left|\frac{\partial u}{\partial z}\right| \approx p\rho^2|z|^{-2} \lesssim p^{-3},$$
$$\left|\frac{\partial u}{\partial \rho}\right| \approx p\rho|z|^{-1} \lesssim p^{-1},$$
$$|\vec{\nabla}F_c/F_c| \lesssim p^{-1}.$$

In the second case $|u|$ is large $\approx p$, therefore Eqs. (A1) and (A2) apply, giving

$$|F_c'/F_c| \approx p^{-1}.$$

Estimating the partial derivatives of u we note, that $|z|$ must be of order ρ^2, giving

$$\left|\frac{\partial u}{\partial z}\right| \lesssim p^{-1}, \quad \left|\frac{\partial u}{\partial \rho}\right| \lesssim 1.$$

Therefore, we obtain

$$|\vec{\nabla}F_c/F_c| \lesssim p^{-1}.$$

Finally, in the third case, $|u|\gtrsim p^2$; we again apply Eqs. (A1) and (A2), getting

$$|F_c'/F_c| \lesssim p^{-2}.$$

Noting that now we must have $|z|\lesssim\rho$, we get

$$\left|\frac{\partial u}{\partial z}\right| \approx p, \quad \left|\frac{\partial u}{\partial \rho}\right| \approx p, \quad \left|\frac{\vec{\nabla}F_c}{F_c}\right| \lesssim p^{-1}.$$

Therefore, in the whole region 4 we have

$$|\vec{\nabla}F_c/F_c| \lesssim p^{-1}.$$

Considering the whole configuration space, we get the following behavior of $|\vec{\nabla}F_c/F_c|$:

$$\left|\frac{\vec{\nabla}F_c}{F_c}\right| \lesssim p, \quad \text{region 1;}$$
$$\lesssim 1, \quad \text{region 2;}$$
$$\approx 1, \quad \text{region 3;}$$
$$\lesssim p^{-1}, \quad \text{region 4.}$$

APPENDIX B. ESTIMATES OF THE DERIVATIVES OF χ_0

It is straightforward to establish the following expressions for the derivatives of χ_0, setting $Ep^{-1}\approx 1$,

$$\frac{\partial\chi_0}{\partial z} \approx -V_1, \quad \frac{\partial^2\chi_0}{\partial z^2} \approx -V_1' z r^{-1},$$
$$\frac{\partial}{\partial z}\frac{\partial\chi_0}{\partial\rho} = \frac{\partial}{\partial\rho}\frac{\partial\chi_0}{\partial z} \approx -V_1'\rho r^{-1},$$
$$\frac{\partial\chi_0}{\partial\rho} \approx -\rho\int_{-\infty}^{z} V_1'(\rho^2+\xi^2)^{-1/2}d\xi, \tag{B1}$$
$$\frac{\partial^2\chi_0}{\partial\rho^2} \approx -\int_{-\infty}^{z} V_1'(\rho^2+\xi^2)^{-1/2}d\xi$$
$$-\rho^2\int_{-\infty}^{z} V_1''(\rho^2+\xi^2)^{-1}d\xi$$
$$+\rho^2\int_{-\infty}^{z} V_1'(\rho^2+\xi^2)^{-3/2}d\xi, \tag{B2}$$

where $V_1' \equiv dV_1/dr$, $V_1'' \equiv d^2V_1/dr^2$, and under all integrals the argument of V_1' and V_1'' is $(\rho^2+z^2)^{1/2}$. To estimate the above derivatives we take for the screened potential V the exponential model[11]

$$V=-Ze^2r^{-1}e^{-\lambda r},$$

where $\lambda=2(\frac{3}{4}\pi)^{-2/3}e^2Z^{1/3}$. Considering the worst case $Z=100$, we get $\lambda=0.038$, $\lambda^{-1}\approx 30$, and

$$V_1=0.73r^{-1}(1-e^{-\lambda r}).$$

For such V_1 the following features of V_1, V_1', and V_1'' can be established:

$$V_1(0)\approx 1.6\,V_1(\lambda^{-1})\approx 0.7\lambda\approx 3\times 10^{-2},$$

$$V_1(r)<0.7r^{-1} \text{ for } r>\lambda^{-1};$$

$$V_1'(0)\approx 1.9V_1'(\lambda^{-1})\approx -0.4\lambda^2\approx 5\times 10^{-4},$$

$$|V_1'(r)|<0.7r^{-2} \text{ for } r>\lambda^{-1};$$

$$V_1''(0)\approx 2.0\,V_1''(\lambda^{-1})\approx 0.2\lambda^3\approx 10^{-5},$$

$$V_1''(r)<1.5r^{-3} \text{ for } r>\lambda^{-1};$$

V_1, $-V_1'$, and V_1'' are very small, positive, decreasing functions, with maximum value at $r=0$, proportional to λ, λ^2, and λ^3, respectively. Similar features can be verified numerically in the case of the modified Thomas-Fermi potential[9,10] used in Sec. IV. Therefore, we may put the following bounds on V_1, $|V_1'|$, and V_1'';

$$V_1<\begin{cases}0.7\lambda,\\ 0.7r^{-1},\end{cases}\quad |V_1'|<\begin{cases}0.4\lambda^2,\\ 0.7r^{-2},\end{cases}\quad V_1''<\begin{cases}0.2\lambda^3, & r<\lambda^{-1}\\ 1.5r^{-3}, & r>\lambda^{-1}.\end{cases} \tag{B3}$$

These bounds give us immediately the estimates for the derivatives of χ_0 with respect to z:

$$\left|\frac{\partial\chi_0}{\partial z}\right|<0.7\lambda,\quad \left|\frac{\partial^2\chi_0}{\partial z^2}\right|<0.7\lambda^2. \tag{B4}$$

The estimate of $|\partial\chi_0/\partial\rho|$ we get from Eqs. (B1) and (B3) setting $z=\infty$ for the worst case. We get

$$\left|\frac{\partial\chi_0}{\partial\rho}\right|<\begin{cases}1.5[1-(1-\lambda^2\rho^2)^{1/2}]+0.4\lambda^2\rho\ln\left(\dfrac{1+(1-\lambda^2\rho^2)^{1/2}}{1-(1-\lambda^2\rho^2)^{1/2}}\right)<2\lambda, & \rho<\lambda^{-1},\\ 1.5\rho^{-1}, & \rho>\lambda^{-1}.\end{cases} \tag{B5}$$

Therefore, we get

$$\left|\frac{\partial\chi_0}{\partial\rho}\right|<2\lambda. \tag{B6}$$

Equation (B5) can be also used for estimating $|\rho^{-1}\partial\chi_0/\partial\rho|$. Now, the term containing logarithm plays the most important role, and restricting ρ from below $\rho\geq 0.1$, we get

$$\left|\rho^{-1}\frac{\partial\chi_0}{\partial\rho}\right|<5.4\lambda^2. \tag{B7}$$

Finally, the second derivative with respect to ρ is estimated from Eqs. (B2) and (B3). We evaluate separately the positive and negative integrals, setting $z=\infty$ in each of them, and then take the greater modulus of the positive and negative contribution as the estimate. The result is

$$\left|\frac{\partial^2\chi_0}{\partial\rho^2}\right|<\begin{cases}5.4\lambda^2, & 0.1\leq\rho<\lambda^{-1}\\ 1.5\rho^{-2}, & \lambda^{-1}<\rho.\end{cases} \tag{B8}$$

Therefore

$$\left|\frac{\partial^2\chi_0}{\partial\rho^2}\right|<5.4\lambda^2 \text{ for } 0.1\leq\rho. \tag{B9}$$

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