

PHOTODETACHMENT MICROSCOPE WITH A REPULSIVE COULOMB FIELD

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Аннотация. Исследование электронных волн с высокой степенью когерентности, образующихся в процессе фоторазрушения отрицательного иона, является физической основой для развития электронной голографии высокого разрешения. Интерференционная картина рассматривается в квазистационарном приближении. В полуклассическом приближении уходящая волна описывается амплитудой, медленно меняющейся вдоль траектории. Квантовое описание фотоотрыва электронов сформулировано на основе соответствующего неоднородного уравнения Шредингера. Его асимптотическое решение выражено через функцию Грина, которая имеет точное аналитическое представление для однородного электрического поля и кулоновского поля. Показано, что кулоновское поле отталкивания эффективно увеличивает область интерференции на малых расстояниях от отрицательного иона.

Ключевые слова: Электронные волны, фотоотрыв, уравнение Шредингера, функция Грина, кулоновское поле, квазиклассическое приближение.

Abstract. The investigation of electronic waves with high degree of coherence in the photodetachment of a negative ion gives a physical basis to develop the holographic electronic microscopy with high resolution. The interference pattern is considered in the framework of steady-state wave approximation. In semiclassical approximation, an outgoing wave is described by the amplitude slowly varying along a trajectory. Quantum description of electron photodetachment from negative ion is formulated on the basis of the inhomogeneous Schrödinger equation. Its asymptotic solution is expressed in terms of the Green function that has exact expression for the homogeneous electric field and the Coulomb field. It is demonstrated that repulsive Coulomb field is effective for extension of the interference pattern at a short distance from an ion.

Keywords: Electronic waves, photodetachment, Schrödinger equation, Green function, Coulomb field, semiclassical approximation.

INTRODUCTION

In recent years an increasing attention is focused on the physical effects of quantum interference. The principal problems of quantum measurements and some perspective applications became the basic stimulus to investigate this area of researches [1, 2]. The electronic waves with high degree of coherence became a basis for progress in electronic microscopy with high resolution and for developing a holography with a low energy. This circumstance opens an opportunity for non-destructive observation with the help of a new tool for nanometer scale objects.

Earlier, the analytical theory was developed to explain experimental results for photodetachment microscope where electrons were detached from negative ions in a homogeneous electric field [3–6]. The advantage of this theory is exact and compact formulation of the result. The quantum

interference is taken into account in a three-dimensional space, including a caustic surface and shadow zone. The idea of the photodetachment microscope was proposed in [7, 8]. The principle of this type of microscope is based on two fundamental effects. The first effect is the Wigner law for the electron photodetachment cross section of a negative ion in the vicinity of a threshold. According to this law, the partial cross section for electron photodetachment into a final state with momentum quantum number l is an exponential function of the photoelectron energy ε :

$$\sigma \sim \alpha \varepsilon^{l+1/2}. \quad (1)$$

For a negative halogen ion the initial electron state has orbital quantum number $l = 1$, and the possible angular moments of the final states are equal to 0 or 2. The corresponding cross sections behave as well as $\varepsilon^{1/2}$ and $\varepsilon^{5/2}$. The partial channel of photodetachment into final s -state dominates close to the threshold, and this state is

described by a spherical outgoing wave. Multiphoton detachment near the threshold may be a source of coherent electrons also [9]. The second effect is an interference of coherent electronic waves at the propagation of monoenergetic electronic beam in an electric field along different paths. For example, in a homogeneous electric field two different trajectories come from the initial point to the same final point. This dynamics is similar to the particle motion, starting under the angle to the horizon in the homogeneous gravitation field. For the case, when the initial altitude is non zero, and for a given momentum, we have two different ways that hit the same final target in accordance with two different elevation angles. The time of classical flight for these two trajectories are different, but for propagation of steady-state waves the interference conditions are well defined. The purpose of this paper is a complete description of the electron wave interference after the process of a negative ion photodetachment in the static repulsive Coulomb field. In this context, the process in a homogeneous electric field can be interpreted as a limiting case. The combination of fields, for another case of electron wave propagation in photoionization of H atom from $n=2$ state in uniform electric field, has been investigated by semiclassical method and quantum mechanical approach [10, 11]. Nearly the same phenomena, but for xenon atom, was observed experimentally in [12] with only qualitative semiclassical description.

SEMICLASSICAL THEORY

In further consideration we assume that previous results of photodetachment cross section calculations in the presence of external static electric field are known [13–17]. All attention is concentrated on the interference of electronic waves and photocurrent density in space. The distance r in the vicinity of negative ion where electron motion is approximately free of external electric field action is determined by inequality $1/p \ll r \ll p^2/2F$, where p is electron momentum in the moment of detachment, and F is electric field strength (in our paper we use an atomic system of units where $e = m_e = \hbar = 1$). Physical meaning of the formulated condition is the work of electric field at the electron wave length distance is less than its kinetic energy. This excludes electron energies too close to the threshold. Then the overall picture of the interference

phenomena can be described in the framework of the semiclassical approximation [18-20]. In this approach the wave propagation is described with the help of amplitude, slowly varying along a trajectory. The waves going by different paths demonstrate interference. The total electron flux at a fixed point of observation is proportional to the square of partial wave amplitudes along different trajectories. The result can be formulated mathematically in the following way [21]. The Schrödinger equation for a particle in an electric field with a potential $U(q)$ has the form

$$i \frac{\partial \psi(q, t)}{\partial t} = -\frac{\Delta}{2} \psi(q, t) + U(q) \psi(q, t), \quad (2)$$

where ψ is a wave function. We assume the initial condition for the wave function of the form

$$\psi|_{t=0} = \varphi(q) e^{iS(q)}, \quad (3)$$

and $S(q)$ is a classical action. Smoothly varying function $\varphi(q)$ is differed from zero only inside a bounded space. Here the classical Hamilton equations are

$$\dot{q} = \frac{\partial H}{\partial p}, \dot{p} = -\frac{\partial H}{\partial q}, \quad (4)$$

where the Hamilton function is

$$H = \frac{p^2}{2} + U(q). \quad (5)$$

The initial point in the phase space is (p_i, q_j) , and the action S_j along a trajectory, started at the point (p_i, q_j) , is

$$S(Q, t) = S(q_j) + \int_0^t L d\tau, \quad L = \frac{\dot{q}^2}{2} - U(q), \quad (6)$$

where L is the Lagrange function.

The solution to Eq. (2) with the initial condition of Eq. (3) has the asymptotic form

$$\psi(Q, t) = \sum_j \phi(q_j) \left| \frac{DQ}{Dq_j} \right|^{\frac{1}{2}} e^{iS_j(Q, t) - \frac{i\pi}{2} \mu_j}, \quad (7)$$

where DQ / Dq_j is a transformation Jacobian for coordinates along a trajectory. Parameter μ_j is an integer number, named the Maslov index of the j -th trajectory [22]. At a unary contact of a trajectory with caustic surface the phase change is $\pi / 2$, and the Maslov index is equal 1, without a contact with caustic the index $\mu_j = 0$. This situation is typical for homogeneous field, and for the Coulomb potential. The factor $DQ / Dq_j \sim j_{cl}$, where j_{cl} is a classical density of a current.

The quantum formula for electron density of a current gives

$$\mathbf{j} = \frac{i}{2}(\psi \nabla \psi^* - \psi^* \nabla \psi) \approx |\psi|^2 \nabla S. \quad (8)$$

We take the phase dependence of a wave function in the semiclassical approximation as a classical action S . It follows from the Eq. (8) that for two different trajectories coming to the same final point the current can be written down in the form

$$j \sim j_{cl} \left| e^{iS_1 - \frac{i\pi}{2}\mu_1} + e^{iS_2 - \frac{i\pi}{2}\mu_2} \right|^2. \quad (9)$$

If classical current j_{cl} is known, to obtain a correct asymptotic formula for the current density j it is essential to determine S_1, S_2, μ_1, μ_2 . For the first trajectory without a contact with a caustic surface the parameter $\mu_1 = 0$, and for the second trajectory the index $\mu_2 = 1$. As a result, we have

$$j \sim j_{cl}(1 + \cos \alpha), \quad (10)$$

where $\alpha = S_1 - S_2 + \pi/2$. Eq. (10) describes the interference pattern with a number of bright and dark rings. However, at the caustic surface a non physical singularity is predicted because of a contact of two trajectories, starting from the same point with a fixed energy of electrons and different initial directions.

QUANTUM-MECHANICAL APPROACH

The complete experimental picture can be reproduced by the advanced quantum theory. We describe the photodetachment of electron from a negative ion by a weak monochromatic laser field with linear polarization. The influence of laser field can be assumed small and is considered by the perturbation theory. Therefore, the photodetachment of electron is a steady-state process. An initial state of a negative ion is only slightly modified by photocurrent. The electron interaction with a laser field can be written down in the dipole approximation as [23]

$$W = w \exp(-i\omega t) + c.c., \quad w = -\frac{iA}{c}(\mathbf{e}\nabla), \quad (11)$$

where ω is a frequency of the absorbed photon, A is an amplitude of the vector potential, c is the speed of light in vacuum, \mathbf{e} is a unit vector of polarization (we assume polarization is linear). The equation for the quasi-steady outgoing wave function ψ in a final state with the energy $E = E_i + \omega$ in the first order of perturbation theory has a form [6]

$$\left(\frac{\nabla^2}{2} - U(\mathbf{r}) + E \right) \psi = w \psi_i. \quad (12)$$

Here ψ_i is the stationary wave function of an initial electron state with the energy E_i in a negative ion, $U(\mathbf{r})$ is a static field potential.

For a homogeneous electric field \mathbf{F} directed along the OZ axis, the stationary Green function G_E is the solution to the equation

$$\left(\frac{\nabla^2}{2} + Fz + E \right) G_E(\mathbf{r}, \mathbf{r}_1) = \delta(z - z_1) \delta(x - x_1) \delta(y - y_1), \quad (13)$$

where δ is the Dirac delta-function. The exact expression for the three-dimensional Green function is [24]

$$G_E(\mathbf{r}, \mathbf{r}_1) = \frac{1}{2} \frac{1}{|\mathbf{r} - \mathbf{r}_1|} [\text{Ci}(\alpha_+) \text{Ai}'(\alpha_-) - \text{Ci}'(\alpha_+) \text{Ai}(\alpha_-)], \quad (14)$$

$$\alpha_{\pm} = -\left(\frac{1}{4F^2} \right)^{1/3} [2E + \mathbf{F}(\mathbf{r} - \mathbf{r}_1) \pm F|\mathbf{r} - \mathbf{r}_1|],$$

where $\text{Ai}(\alpha)$ and $\text{Ci}(\alpha)$ are the Airy functions, $\text{Ai}'(\alpha)$ and $\text{Ci}'(\alpha)$ are their derivatives [25]. The current at a large distance r has the form

$$j \approx j_0 \text{Ai}^2 \left[\frac{1}{\lambda_0} \left(\frac{\rho^2}{4z} - a \right) \right], \quad (15)$$

$\lambda_0 = (2F)^{-1/3}$, $a = E/F$, z is the distance between negative ion and the center of screen, ρ is the transverse coordinate. At the caustic surface ($\rho = \rho_{\max} = \sqrt{4zE/F}$) the magnitude of the electronic current remains finite. In the classically accessible area

$$j \approx \frac{\sin^2 \left[\frac{2}{3} \left(\frac{a}{\lambda_0} \right)^{3/2} \left(1 - \rho^2 / \rho_{\max}^2 \right)^{3/2} + \pi / 4 \right]}{\sqrt{1 - \rho^2 / \rho_{\max}^2}}. \quad (16)$$

This expression agrees well with the semiclassical result given by Eq. (9). It should be stressed that correct semiclassical formula (16) can be derived from Eq. (10) only with proper Maslov indexes [26].

In Fig. 1 the density of a photocurrent $j(\rho)$ is plotted for $F = 100$ V/m, $z = 0.5$ m, $E = 0.2$ cm⁻¹ (1 cm⁻¹ = $4.5 \cdot 10^{-6}$ a.u. = $1.239 \cdot 10^{-4}$ eV). It is apparent that the semiclassical approximation reproduces an exact solution far from the caustic surface. The classical result indicates the position

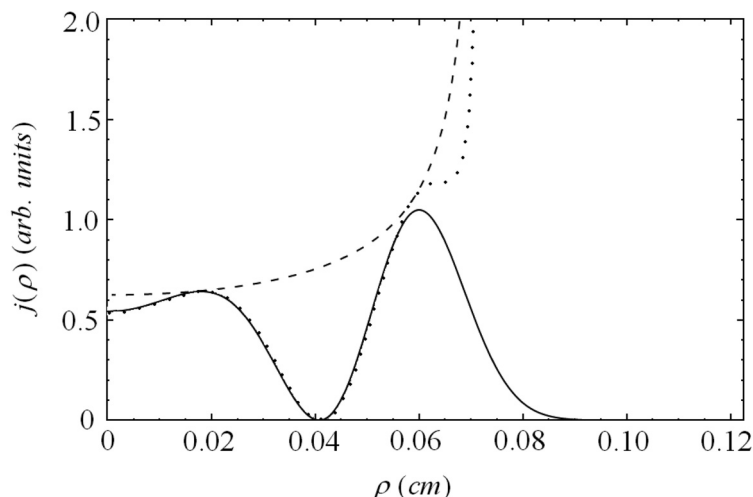


Fig. 1. Transverse density of a photocurrent in a homogeneous field: a dot curve is a classical approximation; dashed curve is a semiclassical result; a continuous curve is a quantum theory calculation

of a caustic but interference pattern with rings of intensity is entirely absent. This result points clearly that classical motion calculations [27] have a very restricted applicability.

In Fig. 2 the change of a photocurrent density along the transverse direction ρ with the growth of the distance z is shown as a shadow graphic. A transversal extension of electron flux is demonstrated during its propagation along the electric field. These calculations and basic formulas give us data for comparison with alternative geometry. It is significant that complete analysis of a uniform field scheme is very useful for calculation of the density close to caustic in more complicated cases [11, 28].

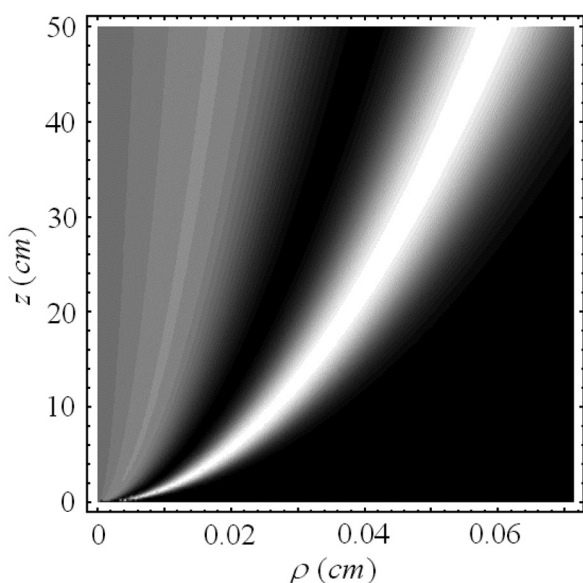


Fig. 2. Variation of density of a photocurrent with a distance to the source

Investigation of other electric field configurations for more effective extension of the interference pattern at a smaller distance is expedient. One of the most interesting cases is an electron photodetachment in the external repulsive Coulomb field as shown in Fig. 3.

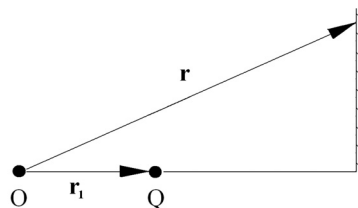


Fig. 3. The mutual position of the repulsive Coulomb center O and a negative ion Q

Analytical representation for the Green function in the Coulomb field with a negatively charged point center is [29]

$$G_E(\mathbf{r}, \mathbf{r}_1) = \frac{2\Gamma(1-i\eta)}{4\pi|\mathbf{r}-\mathbf{r}_1|} \frac{1}{ik} \left(-\frac{\partial}{\partial y} + \frac{\partial}{\partial x} \right) \times \\ \times W_{i\eta, \frac{1}{2}}(-ikx) M_{i\eta, \frac{1}{2}}(-iky) = \quad (17) \\ = -\frac{\Gamma(1-i\eta)}{2\pi|\mathbf{r}-\mathbf{r}_1|} \begin{vmatrix} W_{i\eta, \frac{1}{2}}(-ikx) & M_{i\eta, \frac{1}{2}}(-iky) \\ W'_{i\eta, \frac{1}{2}}(-ikx) & M'_{i\eta, \frac{1}{2}}(-iky) \end{vmatrix}.$$

Here $\eta = -m\alpha/k$, $k = \sqrt{2mE}$, $x = r + r_1 + |\mathbf{r}-\mathbf{r}_1|$, $y = r + r_1 - |\mathbf{r}-\mathbf{r}_1|$, $W_{i\eta, \frac{1}{2}}$ and $M_{i\eta, \frac{1}{2}}$ are the

Whittaker functions, $\Gamma(v)$ is gamma-function [30], vector \mathbf{r}_1 connects a repulsive center and a negative ion.

At a large distance r from the Coulomb center, the radial density of a current j_r has the asymptotic form

$$j_r = \frac{1}{m} \operatorname{Im} \left[\psi^* \frac{\partial \psi}{\partial r} \right] \approx \frac{k}{m} \operatorname{Im} [\psi^* \psi] = \frac{k}{m} |A G(\mathbf{r}, \mathbf{r}_1)|^2 \sim \frac{1}{r^2} \left| M'_{i\pi/2}(-iky) - M_{i\pi/2}(-iky) \right|^2. \quad (18)$$

For a larger r the term with derivative can be neglected. The multiplier $1/r^2$ is nearly constant at a large distance from the Coulomb center. It is instructive to consider the density in a transverse direction ρ , where

$$j(\rho) \sim \left| M_{i\pi/2}(-iky) \right|^2. \quad (19)$$

From the structure of the Green function (see Eq. (17)), it is clear that one-dimensional equation for the Coulomb potential

$$\frac{d^2 \chi}{dr^2} + \left(k^2 - \frac{2m\alpha}{r} \right) \chi = 0 \quad (20)$$

is principal for accurate development of three-dimensional Green function in the repulsive Coulomb field. For more detailed analyses of Eq. (20) we replace variable: $v = r/\beta$. The new equation is of the form

$$\frac{d^2 \chi}{dv^2} + \left(1 - \frac{Z}{v} \right) \chi = 0, \quad (21)$$

where $\beta = 1/k$, $Z = 2m\alpha$.

The semiclassical solution of the one-dimensional Schrödinger equation in classically inaccessible area ($v < Z$) is [31]

$$\chi(v) = \frac{A}{\sqrt{|p|}} \exp \left(- \int_{r_0}^r p dr \right). \quad (22)$$

In classically accessible area ($v > Z$) we have

$$\chi(v) = \frac{B}{\sqrt{p}} \cos \left(\int_{r_0}^r p dr - \pi/4 \right) \quad (23)$$

The integral is calculated over the classical area, starting from a turning point $r_0 = 2m\alpha/k^2$. The phase shift $\pi/4$ arises as a result of reflection at the classical turning point.

Calculating a phase, where $p(r) = \sqrt{k^2 - 2m\alpha/r}$, we have

$$S(r) = \int_{r_0}^r p(r) dr = kr_0 \left(\sqrt{s(s-1)} - \ln(\sqrt{s-1} + \sqrt{s}) \right), \quad (24)$$

and $s = v/Z = r/r_0$.

For the classically inaccessible region $p(r) = \sqrt{Z/v - 1}$, and

$$S(r) = \int_{r_0}^r p(r) dr = kr_0 \left(s\sqrt{1/s-1} + \arcsin(2s-1) - \pi/2 \right). \quad (25)$$

Then the solution for this region ($v < Z$)

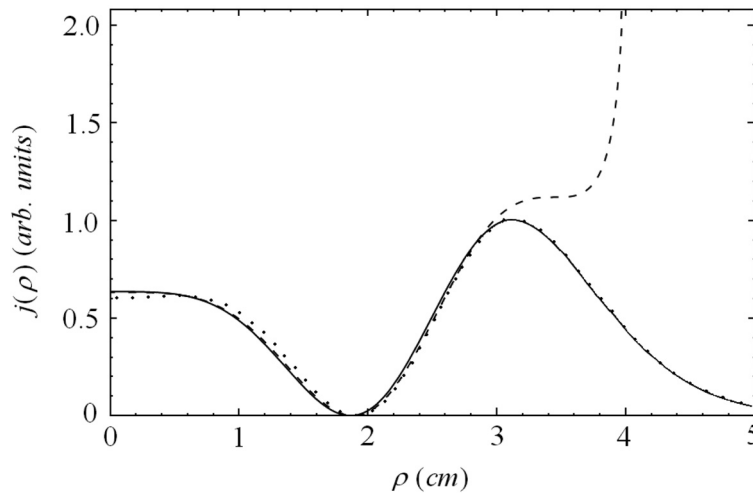


Fig. 4. Density of an electronic current for the following parameters: $z = 5$ cm, $|\mathbf{r}_1| = 2 \times 10^{-4}$ cm, $E = 0.2$ cm $^{-1}$ and the electric field strength near negative ion $F = 100$ V/m. Semiclassical solution is shown by a dotted line, uniform field approximation are points, the exact solution is a continuous line

$$\chi = \frac{C}{\left(\frac{1}{s}-1\right)^{\frac{1}{4}}} \exp\left(-kr_0\left(s\sqrt{\frac{1}{s}-1}-\arcsin(2s-1)+\frac{\pi}{2}\right)\right), \quad (26)$$

and in classically accessible area ($v > Z$)

$$\chi = \frac{C}{\left(1-\frac{1}{s}\right)^{\frac{1}{4}}} \sin\left(kr_0\left(\sqrt{s(s-1)}-\ln\left(\sqrt{s-1}+\sqrt{s}\right)\right)+\frac{\pi}{4}\right). \quad (27)$$

The results of calculations, according to the semiclassical approximation, in comparison with the exact solution are shown in Fig. 4. Evidently, semiclassical approximation is good enough for classically accessible area. In the vicinity of the caustic, the semiclassical approximation tends to infinity, whereas the exact solution remains finite. A uniform field approximation gives a rather good result for all distances and in combination with semiclassical approximation for $\rho < 2$ cm reproduces the exact result.

The space distribution of an electron current density is demonstrated in Fig. 5. The repulsive Coulomb field plays the role of projector and magnifies the initial density dramatically.

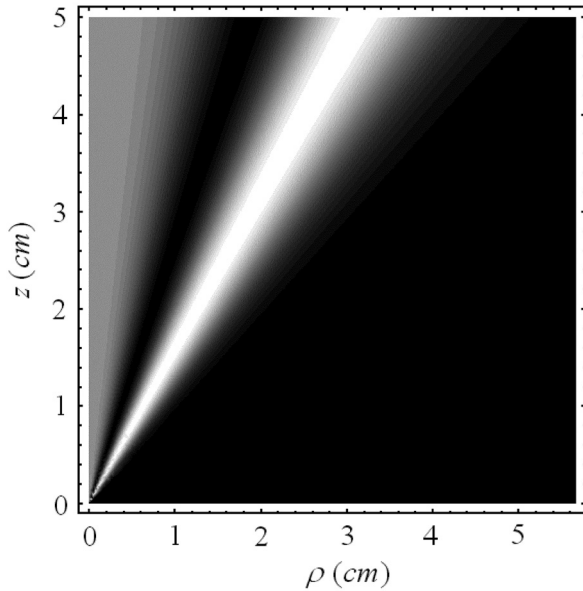


Fig. 5. Variation of a photocurrent density $j(\rho)$ with the growth of z as a function of transverse coordinate ρ

CONCLUSION

Our calculations demonstrate new opportunities for a control of electron waves by a static electric field. Operating with the repulsive Coulomb field, it is possible to produce a multiply magnified

projection of electron flux. For the one-electron wave packets this problem was discussed in [32].

A number of experimental and theoretical investigations were previously concentrated on the case of homogeneous electric field. The interference spot had the size of near micrometer under real experimental conditions. The trajectories are stretched along electric field direction, so in the experiments the distance between the negative ion and the registration plate is approximately one meter. However, the electron wave interference has a universal physical nature and occurs in different electric field configurations. We propose to employ the repulsive Coulomb field, because it is a more effective projection scheme, for the purposes of an electron coherent microscopy. The total analytical solution of the problem is based on the Green function for the Coulomb field and expressed in terms of Whittaker functions. Its asymptotic form allows immediately to calculate a photocurrent. This new experimental geometry, based on nano size electrode technology [33], guarantees an effective expansion of the interference pattern. Inside the central part of the interference area, the pattern may be reproduced with the help of much more simple semiclassical calculations. We assume that the best realization of a negative ion photodetachment microscope is the two-field scheme with a combination of the homogeneous electric field and the repulsive Coulomb field.

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