

Zeitschrift: Helvetica Physica Acta
Band: 70 (1997)
Heft: 1-2

Artikel: Multiphoton ionization of the delta-function atom
Autor: Robustelli, D. / Saladin, D. / Scharf, G.
DOI: <https://doi.org/10.5169/seals-117013>

Nutzungsbedingungen

Die ETH-Bibliothek ist die Anbieterin der digitalisierten Zeitschriften. Sie besitzt keine Urheberrechte an den Zeitschriften und ist nicht verantwortlich für deren Inhalte. Die Rechte liegen in der Regel bei den Herausgebern beziehungsweise den externen Rechteinhabern. [Siehe Rechtliche Hinweise.](#)

Conditions d'utilisation

L'ETH Library est le fournisseur des revues numérisées. Elle ne détient aucun droit d'auteur sur les revues et n'est pas responsable de leur contenu. En règle générale, les droits sont détenus par les éditeurs ou les détenteurs de droits externes. [Voir Informations légales.](#)

Terms of use

The ETH Library is the provider of the digitised journals. It does not own any copyrights to the journals and is not responsible for their content. The rights usually lie with the publishers or the external rights holders. [See Legal notice.](#)

Download PDF: 29.03.2025

ETH-Bibliothek Zürich, E-Periodica, <https://www.e-periodica.ch>

Multiphoton Ionization of the Delta-Function Atom

By D.Robustelli, D.Saladin and G.Scharf

Institut für Theoretische Physik der Universität Zürich
Winterthurerstr. 190, CH-8057 Zürich, Switzerland

(3.VI.1996)

Abstract We study the one-dimensional and three-dimensional delta-function atom in an electric field with sinusoidal time dependence. Using the exact continuum states of the one-dimensional model we calculate the spectra of the photoelectrons. The spectra show a series of very high and sharp multiphoton peaks. The ponderomotive shift of these peaks is analysed. The three-dimensional problem is reduced to an integro-differential equation in time which can be converted into a Volterra integral equation. The latter is well suited for functional analytic discussion and numerical solution.

1 Introduction

The one-electron atom with an attractive delta-potential is ridiculously simple compared with real atoms, where the work of Walter Hunziker is relevant. Nevertheless, the ridiculous atom has a real counterpart, namely a negative ion such as H^- , where the electron is weakly bound by a short-range potential. If the δ -function atom is put into an electric field with sinusoidal time dependence (frequency ω), it shows a surprisingly rich dynamics. This is illustrated in fig.1 where the ionization probability P of the one-dimensional model is shown as a function of the field strength μ , the latter is measured in terms of the so-called ponderomotive energy

$$U_P = \frac{\mu^2}{2\omega^2}. \quad (1.1)$$

The model has a long history which starts with a paper by Geltman [1] in 1977. Most accurate results for the ionization probability in the one-dimensional case can be

found in [2] from which fig.1 is taken and where further references are given. In the following we complete these previous calculations by computing the energy spectra of the photoelectron. Earlier results for the spectra [3] suffer from an obvious drawback: One has not used the exact continuum states of the delta-function atom, but, instead, Volkov states which were Gram-Schmidt orthogonalized with respect to the ground state of the delta-function atom. This procedure which was suggested by Faisal et al. [4] does not have a quantum mechanical justification, because those continuum states are not eigenstates of a physical observable. For this reason we have computed the electron spectra by projecting on the exact continuum states of the delta-function atom.

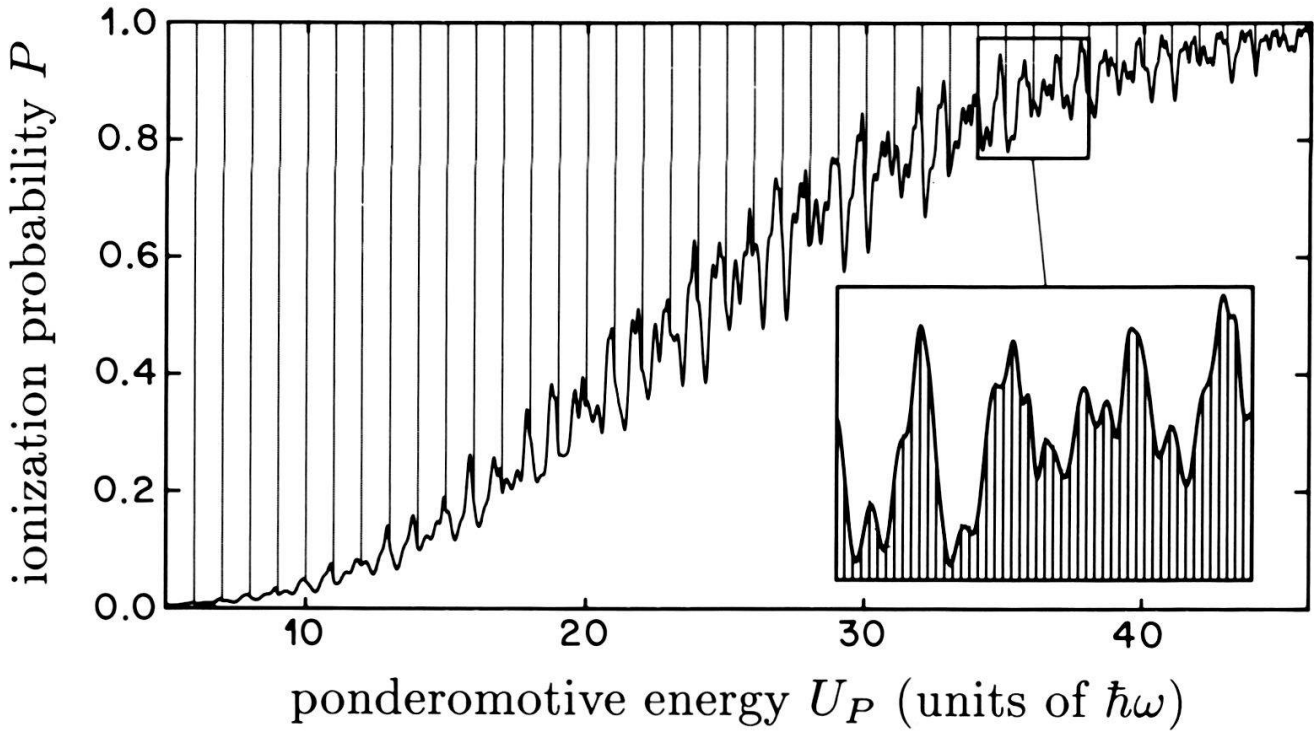


Fig.1 Ionization probability P as a function of $\mu^2/2\omega^3$ for $\omega_0/\omega = 10$ after 10 optical cycles.

In section 3 we consider the three-dimensional model. In this case the delta-potential must be modified by a derivative in order to get a well defined self-adjoint Hamiltonian. The problem can then be reduced to an integro-differential equation in time with weakly singular kernel. In deriving this equation we observe that the three-dimensional point interaction is no longer spherically symmetric in the presence of the electric field, but gets a directional dependence. The integro-differential equation is then converted into a Volterra integral equation of a similar form as in the one-dimensional case. This equation was discussed by Guidotti and Hieber [13] in the Banach space of continuous functions (in time) and global existence and uniqueness of the solution was established. Numerical calculations of the ionization probability are in progress.

2 Electron Spectra for the One-Dimensional Model

In this section we study the motion of an electron in an attractive one-dimensional δ -function potential subject to an external sinusoidal electric field:

$$H(t) = H_0 + H_1(t) \quad (2.1)$$

where

$$H_0 = p^2/2m - \alpha\delta(x) \quad (2.2)$$

with $\alpha > 0$, and

$$H_1(t) = E(t)x = -\mu x \cos \omega t. \quad (2.3)$$

We use units so that $\hbar^2/2m = 1 = \alpha$. Then H_0 has a unique bound state

$$\psi_0(x) = e^{-|x|/2}/\sqrt{2} \quad (2.4)$$

with binding energy $E = -\omega_0 = -1/4$, which we take as initial state at $t = 0$. The continuum states of H_0 are best obtained by means of scattering theory on the line [5]. One defines Jost solutions

$$H_0 f_{\pm}(k, x) = k^2 f_{\pm}(k, x) \quad (2.5)$$

by their asymptotic behaviour

$$f_{\pm} \sim e^{\pm ikx}, \quad x \rightarrow \pm\infty. \quad (2.6)$$

They are given by

$$f_+(k, x) = \begin{cases} e^{ikx}, & \text{if } x > 0 \\ \left(1 + \frac{1}{2ik}\right)e^{ikx} - \frac{1}{2ik}e^{-ikx} & \text{for } x < 0 \end{cases} \quad (2.7)$$

$$f_-(k, x) = \begin{cases} -\frac{1}{2ik}e^{ikx} + \left(1 + \frac{1}{2ik}\right)e^{-ikx}, & \text{if } x > 0 \\ e^{-ikx}, & \text{for } x < 0 \end{cases} \quad (2.8)$$

and

$$T(k) = \frac{2ik}{2ik + 1} \quad (2.9)$$

is the transmission coefficient. The spectral decomposition of H_0 now assumes the following form [5]

$$\begin{aligned} \delta(x - y) = & \frac{1}{4\pi} \int_{-\infty}^{+\infty} dk |T(k)|^2 [f_+(k, y)^* f_+(k, x) + \\ & + f_-(k, y)^* f_-(k, x)] + \psi_0(y)\psi_0(x). \end{aligned} \quad (2.10)$$

This is the basis for calculating the electron spectrum.

To solve the time-dependent Schrödinger equation for $H(t)$, we use the fact that the propagator (Green's function) U_t corresponding to

$$K_0(t) = -\partial^2/\partial x^2 + E(t)x \quad (2.11)$$

is explicitly known [6]. It is the solution of

$$i \frac{\partial}{\partial t} U_t = K_0(t) U_t \quad (2.12)$$

with $U_0 = 1$. Following [6] one makes the following product ansatz

$$U_t = e^{-ia(t)} e^{-ib(t)x} e^{-ic(t)p} e^{-itp^2}. \quad (2.13)$$

It is straightforward to show that (2.12) is satisfied by choosing $a(t)$, $b(t)$ and $c(t)$ as follows

$$b(t) = \int_0^t E(s) ds, \quad a(t) = \int_0^t b(s)^2 ds \quad (2.14)$$

$$c(t) = -2 \int_0^t b(s) ds. \quad (2.15)$$

The propagator (2.13) is usually called Volkov propagator [7]. Taking into account (2.12), we see that the Schrödinger equation

$$i \frac{\partial \psi}{\partial t} = (K_0(t) - \delta) \psi \quad (2.16)$$

is equivalent to the following integral equation (Duhamel formula)

$$\psi_t = U(t, 0) \psi_0 + i \int_0^t U(t, s) \delta \psi_s ds \quad (2.17)$$

where $U(t, s) = U_t U_s^{-1}$. Using (2.14-15) it is easy to express U as an integral operator

$$(U(t, s) \psi)(x) = \frac{e^{-i[b(t)x + \pi/4]}}{\sqrt{4\pi(t-s)}} e^{-ia(t,s)} \int_{-\infty}^{\infty} dy \psi(y) e^{ib(s)y} \exp i \frac{[c(t,s) - x + y]^2}{4(t-s)} \quad (2.18)$$

$$\text{where } a(t, s) \stackrel{\text{def}}{=} a(t) - a(s), \quad c(t, s) \stackrel{\text{def}}{=} c(t) - c(s). \quad (2.19)$$

Taking as initial condition $\psi_0(x) = e^{-|x|^2/2}/\sqrt{2}$, we see that due to the delta function in (2.17), only the value of ψ_s at $x = 0$ contributes at the r.h.s of (2.17). Let us introduce the function

$$\Phi(t) \stackrel{\text{def}}{=} \sqrt{2} \psi_t(0) e^{ia(t)}, \quad \Phi(0) = 1. \quad (2.20)$$

Setting, then, $x = 0$ in (2.18), we get the following (weakly) singular Volterra equation for Φ :

$$\Phi(t) = e^{ic(t)^2/4t} \bar{w}(t) + \sqrt{\frac{i\omega_0}{\pi}} \int_0^t ds \frac{\Phi(s)}{\sqrt{t-s}} \exp i \frac{c(t,s)^2}{4(t-s)}, \quad (2.21)$$

where $\sqrt{i} \stackrel{\text{def}}{=} \exp[i\pi/4]$. Note that $c(0) = 0$ and the existence of $\dot{c}(0)$ imply that

$$\lim_{t \rightarrow 0} \frac{c^2(t)}{t} = \lim_{s \rightarrow t} \frac{c(t,s)^2}{t-s} = 0.$$

Hence $1/\sqrt{t-s}$ is the only singularity in (2.21). Above,

$$\bar{w}(t) = \frac{1}{2} \left[w(z_+(t)) + w(z_-(t)) \right], \quad (2.22)$$

where

$$z_{\pm}(t) = \sqrt{it} \left(i\sqrt{\omega_0} \pm \frac{c(t)}{2t} \right), \quad \text{and} \quad (2.23)$$

$$w(z) = e^{-z^2} \operatorname{erfc}(-iz) \quad (2.24)$$

is the complex error function [8].

Let Φ denote the unique [9] solution of (2.21), then the wave function at time t is obtained from (2.17)

$$\begin{aligned} \psi_t(x) &= f_t(x) + \frac{1}{\sqrt{4\pi}} e^{-i(b(t)x - \pi/4)} \int_0^t ds \frac{\psi_s(0)}{\sqrt{t-s}} \\ &\quad \times \exp \left(\frac{i}{4(t-s)} [x - c(t,s)]^2 \right). \end{aligned} \quad (2.25)$$

Here

$$\begin{aligned} f_t(x) &= (2\pi i)^{-1/2} e^{-ib(t)x} \sum_{\pm} \int_0^{\infty} dz \exp(-\sqrt{t}z) \\ &\quad \times \exp \left[i \left(z \pm \frac{c-x}{2\sqrt{t}} \right)^2 \right] \end{aligned} \quad (2.26)$$

$$b(t) = \int_0^{\infty} E(s) ds = -\frac{\mu}{\omega} \sin \omega t \quad (2.27)$$

$$c(t,s) = -2 \int_s^t b(s') ds' \quad (2.28)$$

and $\psi_s(0)$ is the solution of the Volterra integral equation (5) specialized to $x = 0$. The latter is solved numerically by the methods described in ref.[2]. The numerical error in the code is under complete control.

The scalar products

$$a_{\pm}(k) = \int_{-\infty}^{+\infty} dy f_{\pm}(k, y)^* \psi_t(y) \quad (2.29)$$

can be analytically calculated from (2.7, 8) and (2.25). The calculation is lengthy but straightforward and leads to the following result:

$$a_{\pm}(k) = J^{(1)} + J_{\pm}^{(2)} \pm J_1^{(3)} \pm J_2^{(3)} \quad (2.30)$$

where

$$J^{(1)} = \frac{2\sqrt{2}e^{-itk^2}}{1 + 4k^2} \quad (2.31)$$

$$J_{\pm}^{(2)} = \frac{i}{\sqrt{2}} \int_0^t ds \Phi(s) \exp\left(i((s-t)k^2 \mp ic(s)k)\right) \quad (2.32)$$

$$J_1^{(3)} = \frac{1}{4k\sqrt{i}} \int_0^t ds \Phi(s) \sum_{\pm} \pm E\left(\frac{c(s) \pm 2k(t-s)}{\sqrt{2\pi(t-s)}}\right) \exp[-ik^2(t-s) \pm ikc(s)] \quad (2.33)$$

$$J_2^{(3)} = \frac{1}{4k\sqrt{i}} \int_0^t ds \Phi(s) \sum_{\pm} \pm E\left(\frac{c(s) \mp 2k(t-s)}{\sqrt{2\pi(t-s)}}\right) \exp[-ik^2(t-s) \pm ikc(s)] \quad (2.34)$$

Here

$$E(z) = C(z) + iS(z) \stackrel{\text{def}}{=} \int_0^z dt \exp\left(\frac{i}{2}\pi t^2\right) \quad (2.35)$$

is the complex Fresnel integral [8]. The final time t has been chosen to be a multiple of the period of the electric field, so that $b(t) = 0 = c(t)$.

Now we want to discuss the main features of the resulting photoelectron probability distributions

$$P(k) = |a_+(k)|^2 + |a_-(k)|^2. \quad (2.36)$$

We always plot this as a function of the energy $E = k^2$. In fig.2 a typical spectrum is shown. Although the qualitative picture of the equidistant multiphoton peaks agrees with the previously published spectra [3], there is a great quantitative difference: Our peaks are about a hundred times higher and more narrow! Apparently this is a consequence of projecting on the exact continuum states. The wrong continuum states give rise to a considerable broadening of the peaks. It is a remarkable feature that such a clean multiphoton picture is provided by a model with a purely classical radiation field.

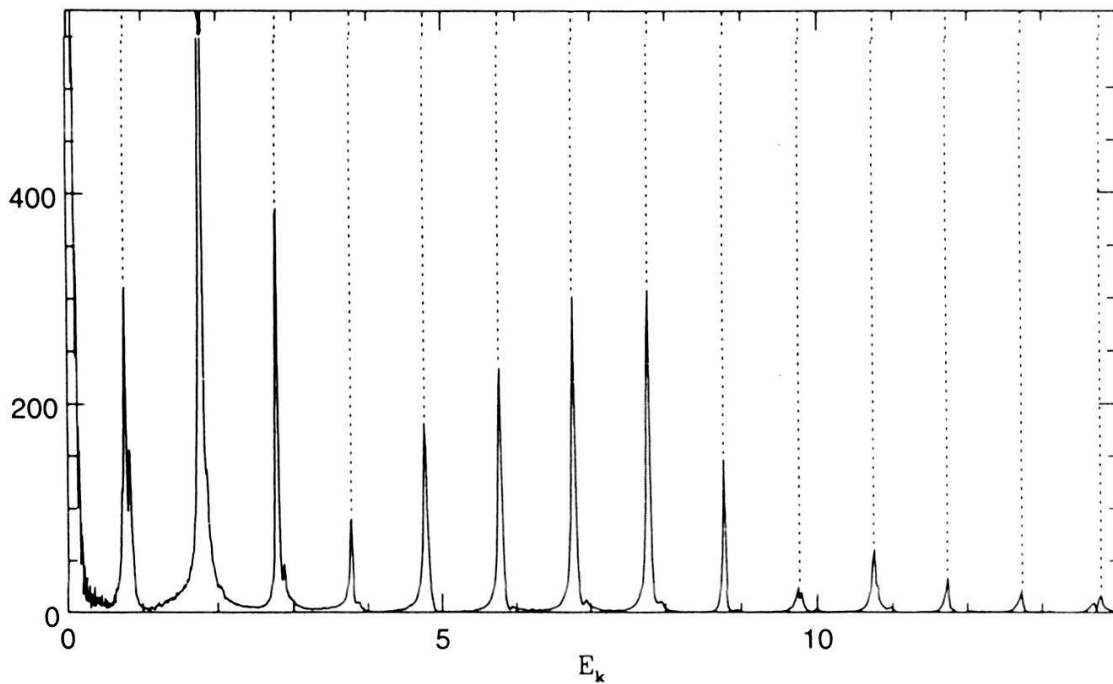


Fig.2. Spectrum for $\omega_0/\omega = 3.5$ and $\mu = 0.0511$ at $t = 30/2\pi\omega$. The energy $E_k = k^2$ is in units $\hbar\omega$. The dotted lines give the positions $n\omega - U_P$ after ponderomotive shift.

The positions of the peaks varies with the field strength μ . The peaks are shifted down from the multiphoton energies $n\omega$ by the ponderomotive energy $U_P = \mu^2/2\omega^2$, apart from the threshold peak at $E = 0$ (fig.3). The classical explanation of this is that the ionized photoelectron has to have the quiver energy U_P in addition to the absorbed photonic energy $n\omega$. Hence the energy left in the δ -atom is $n\omega - U_P$ [10]. The true quantum mechanical explanation is provided by a semiclassical theory of the model [11]. In the path-integral language there is interference between the contribution of the bound electron and the ionization paths. The latter are complex non-classical paths which describe the time-dependent tunnelling [11].

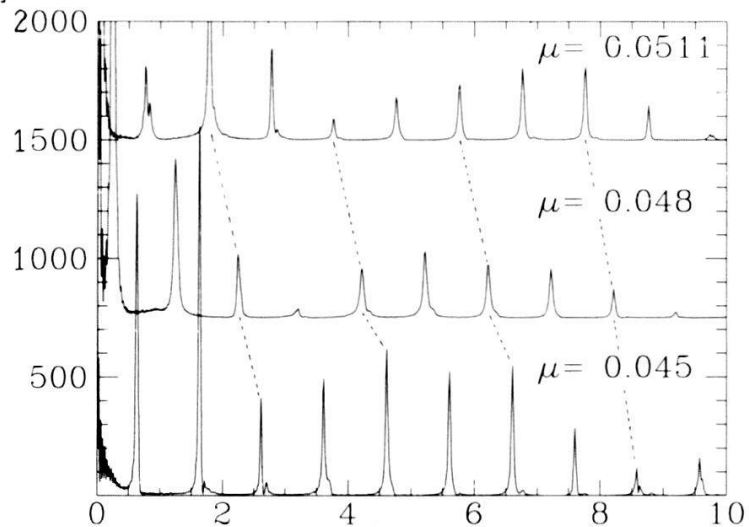


Fig.3. Ponderomotive shifts $\mu^2/2\omega^2$ of the electron spectra for three values of the field strength (other parameters as in Fig.2).

3 The Three-Dimensional Delta Function Atom

The three-dimensional Schrödinger equation of an electron moving in a time-dependent electric field $\vec{E}(t)$, which is constant in space,

$$i \frac{\partial}{\partial t} \psi(t, \vec{x}) = (-\Delta + \vec{E}(t) \cdot \vec{x}) \psi(t, \vec{x}), \quad \hbar = 2m = 1, \quad (3.1)$$

is again solved by the Volkov propagator (2.13). The only difference is that $\vec{b}(t)$ (2.14) and $\vec{c}(t)$ (2.15) are now three-vectors. If, in addition, the electron feels a binding potential $V(\vec{x})$, the corresponding Schrödinger equation can again be converted into an inhomogeneous linear integral equation by means of the Duhamel principle:

$$\psi_t = U_0(t, 0) \psi_0 - i \int_0^t U_0(t, \tau) V \psi_\tau d\tau. \quad (3.2)$$

Let us introduce the quantities

$$e^{ia(t)} e^{i\vec{b}(t)\vec{x}} \psi_t(\vec{x}) = \varphi_t(\vec{x}) \quad (3.3)$$

$$\begin{aligned} e^{ia(t)} e^{i\vec{b}(t)\vec{x}} U_0(t, 0) \psi_0 &= \exp \left[-i \left(\vec{c}(t) \vec{p} + t \vec{p}^2 \right) \right] \psi_0 \\ &= f_t(\vec{x}). \end{aligned} \quad (3.4)$$

If $V = V(\vec{x})$ is a regular potential, the multiplication operator $\exp[i\vec{b}\vec{x}]$ commutes with V and, then, ψ_τ in the integral term of (3.2) goes over into φ_τ (3.3). However, we are going to consider the singular 3-dimensional "δ-potential" [12]

$$V = \frac{1}{\alpha} \delta(\vec{x}) \frac{\partial}{\partial x} \left(x \cdot \right), \quad x = |\vec{x}|, \quad \alpha = \text{const}, \quad (3.5)$$

that does not have this commuting property, in fact

$$\begin{aligned} V_\tau(\vec{x}) &\stackrel{\text{def}}{=} e^{i\vec{b}(\tau)\vec{x}} V e^{-i\vec{b}(\tau)\vec{x}} \\ &= \frac{1}{\alpha} \delta(\vec{x}) \left[\frac{\partial}{\partial x} \left(x \cdot \right) - i\vec{b}(\tau)\vec{x} \right]. \end{aligned} \quad (3.6)$$

If this operates on wave functions which are continuous at $\vec{x} = 0$, the additional term $\vec{b}\vec{x}$ gives 0 due to the δ-distribution. But we must also consider wave functions with an $1/x$ singularity, for example the unique bound state ψ_0 of

$$(-\Delta + V) \psi_0 = E_0 \psi_0, \quad (3.7)$$

which is given by

$$\psi_0 = N \frac{e^{-4\pi\alpha x}}{x}, \quad \alpha > 0 \quad (3.8)$$

$$E_0 = -(4\pi\alpha)^2. \quad (3.95)$$

For $N = \sqrt{2\alpha}$, $\psi_0(\vec{x})$ is normalized in $L^2(\mathbf{R}^3)$. On such functions the last term in (3.6) is not well defined, because the limit of $\vec{x}/x$ for $\vec{x} \rightarrow 0$ depends on the direction. Consequently, the presence of the electric field requires a more precise definition of the zero-range potential (3.5). This subtlety has been overlooked in previous work [4]. We shall postulate that the limit $\vec{x} \rightarrow 0$ in V is to be taken along a fixed direction $\vec{e} = \vec{x}/x$, thus

$$(V_\tau f)(\vec{x}) = \frac{1}{\alpha} \delta(\vec{x}) \left[\frac{\partial}{\partial x}(xf) - i\vec{b}(\tau) \cdot \vec{e}xf \right]_{\vec{x} \rightarrow 0}. \quad (3.10)$$

In this way the 3-dimensional δ -potential has obtained a directional dependence specified by the unit vector $\vec{e}$. As a consequence, the method of self-adjoint extension for introducing the point interaction as described in [12] cannot be applied here.

The p -dependent exponentials in (3.4) define the following integral operator in x -space

$$\left(\exp \left[-i \left((t - \tau) \vec{p}^2 + \vec{c}(t, \tau) \cdot \vec{p} \right) \right] f \right)(\vec{x}) = \int d^3y G(t, \tau, \vec{x} - \vec{y}) f(\vec{y}), \quad (3.11)$$

with a kernel given by

$$G(t, \tau, \vec{x}) = \left(4\pi i(t - \tau) \right)^{-3/2} \exp \left[\frac{i}{4(t - \tau)} \left(\vec{x} - \vec{c}(t, \tau) \right)^2 \right]. \quad (3.12)$$

Then (3.2) is equivalent to

$$\varphi_t(\vec{x}) = f_t(\vec{x}) - \frac{i}{\alpha} \int_0^t d\tau G(t, \tau, \vec{x}) F(\tau), \quad (3.13)$$

with

$$F(t) = \left[\frac{\partial}{\partial y}(y\varphi_t) - i\vec{b}(t) \cdot \vec{e}y\varphi_t \right]_{\vec{y} \rightarrow 0}. \quad (3.14)$$

To get a closed equation for $F(t)$ (3.14), we multiply (3.13) by x , then operate with $[\partial/\partial x - i\vec{b}\vec{e}]$ according to (3.14) and let $\vec{x} \rightarrow 0$. This gives $F(t)$ on the left hand side. The first term f_t on the right side goes over into a function $u(t)$ that is calculated in the appendix. The integral must be treated with great care.

To see the singular behaviour in

$$F_1(t, \vec{x}) = \int_0^t \frac{d\tau}{(t - \tau)^{3/2}} F(\tau) \exp \left[\frac{i}{4(t - \tau)} \left(\vec{x} - \vec{c}(t, \tau) \right)^2 \right], \quad (3.15)$$

we use the substitution

$$z = \frac{t - \tau}{x^2}, \quad (3.16)$$

yielding

$$F_1(t, \vec{x}) = \frac{1}{x} \int_0^{t/x^2} \frac{dz}{z^{3/2}} F(t - zx^2) \exp \left[\frac{i}{4x^2 z} \left(\vec{x} - \vec{c}(t, t - zx^2) \right)^2 \right]. \quad (3.17)$$

After multiplication by x , the integral, say F_2 can be differentiated with respect to x under the integral and in the upper limit of integration. In the limit $\vec{x} \rightarrow 0$ the following terms survive

$$\begin{aligned} \lim_{\vec{x} \rightarrow 0} \frac{\partial F_2(t, \vec{x})}{\partial x} &= -\frac{2}{\sqrt{t}} F(0) \exp \left[\frac{i}{4t} \vec{c}^2(t) \right] - \int_0^t \frac{d\tau}{\sqrt{t-\tau}} \exp \left[\frac{i}{4(t-\tau)} \vec{c}(t, \tau)^2 \right] \\ &\times \left\{ 2F'(\tau) + \frac{i}{2} \frac{F(\tau)}{(t-\tau)^2} \left(\vec{c}(t, \tau)^2 + 4(t-\tau) \vec{b}(\tau) \cdot \vec{c}(t, \tau) \right) \right\}. \end{aligned} \quad (3.18)$$

It is convenient to transform the term with derivative $F'(\tau)$ by partial integration in the form

$$\int_0^t \frac{d\tau}{\sqrt{t-\tau}} F'(\tau) \left\{ \exp \left[\frac{i}{4(t-\tau)} \vec{c}(t, \tau)^2 \right] - 1 \right\}. \quad (3.19)$$

Then we get

$$\begin{aligned} \lim_{\vec{x} \rightarrow 0} \frac{\partial F_2(t, \vec{x})}{\partial x} &= \frac{-2}{\sqrt{t}} F(0) + \\ &+ \int_0^t \frac{d\tau}{(t-\tau)^{3/2}} F(\tau) \left\{ \exp \left[\frac{i}{4(t-\tau)} \vec{c}(t, \tau)^2 \right] - 1 \right\} - 2 \int_0^t \frac{d\tau}{\sqrt{t-\tau}} F'(\tau), \end{aligned} \quad (3.20)$$

where all integrals separately converge at $t = \tau$.

Next we turn to the directional term $\sim \vec{b} \cdot \vec{c}$. We subtract and add an exponential under the integral (3.15). The integral

$$\int_0^t \frac{ds}{s^{3/2}} \left\{ \exp \left[\frac{i}{4s} (\vec{x} - \vec{c})^2 \right] - \exp \left[\frac{i}{4s} \vec{x}^2 \right] \right\} F(t-s), \quad t - \tau = s$$

remains finite in the limit $\vec{x} \rightarrow 0$, so that, after multiplication by $\vec{b}\vec{x}$, it gives no contribution for $\vec{x} \rightarrow 0$. There is left the integral

$$\begin{aligned} F_3(t, \vec{x}) &= \int_0^t \frac{ds}{s^{3/2}} F(t-s) \exp \left[\frac{i}{4s} \vec{x}^2 \right] \\ &= \frac{2}{x} \int_{\vec{x}^2/4t}^{\infty} \frac{dz}{\sqrt{z}} e^{iz} F \left(t - \frac{\vec{x}^2}{4z} \right) \end{aligned} \quad (3.21)$$

with the $1/x$ singularity again. Here we expand F around $F(t)$. Since the correction term vanishes for $\vec{x} \rightarrow 0$, we obtain in this limit

$$F_3(t, \vec{x}) \rightarrow \frac{2}{x} F(t) \int_0^\infty \frac{dz}{\sqrt{z}} e^{iz} = \frac{2\sqrt{\pi}}{x} F(t) \exp\left[i\frac{\pi}{4}\right]. \quad (3.22)$$

After multiplication by $\vec{b}(t) \cdot \vec{x}$, this leads to the directional term $\sim \vec{b} \cdot \vec{x}/x = \vec{b}\vec{e}$. We take this term on the left side of the resulting integro-differential equation

$$\begin{aligned} F(t) \left(1 - \frac{i}{4\pi\alpha} \vec{b}(t) \vec{e}\right) &= u(t) + \frac{F(0)}{4\pi\alpha\sqrt{i\pi t}} - \\ &- \frac{1}{8\pi\alpha\sqrt{i\pi}} \int_0^t \frac{d\tau}{(t-\tau)^{3/2}} F(\tau) \left\{ \exp\left[\frac{i}{4(t-\tau)} \vec{c}(t, \tau)^2\right] - 1 \right\} \\ &+ \frac{1}{4\pi\alpha\sqrt{i\pi}} \int_0^t \frac{d\tau}{\sqrt{t-\tau}} F'(\tau). \end{aligned} \quad (3.23)$$

The linear integro-differential equation (3.23) can be solved for $F(t)$ and this then gives the wave function of the electron according to (3.14). However, eq.(3.23) is inconvenient, because the last term involving the derivative F' complicates the functional analytic discussion of the equation as well as the actual numerical computation. Indeed, it is a general rule for accurate numerical codes that differentiation must be avoided.

To fulfill this rule we modify eq.(3.23) by a method known from the theory of Abel's integral equations. We multiply (3.23) by $1/\sqrt{x-t}$ and integrate in t from 0 to x . This allows to modify the last term by interchanging the order of integrations

$$\begin{aligned} \int_0^x \int_0^t \frac{d\tau F'(\tau)}{\sqrt{(x-t)(t-\tau)}} &= \int_0^x d\tau F'(\tau) \int_\tau^x \frac{dt}{\sqrt{(x-t)(t-\tau)}} = \\ &= \pi \int_0^x d\tau F'(\tau) = \pi[F(x) - F(0)]. \end{aligned} \quad (3.24)$$

Hence, the derivative is gone. In the integral with $F(\tau)$ we also change the order of integration. Then we get

$$\begin{aligned} \int_0^x \frac{dt}{\sqrt{x-t}} \left(1 - \frac{i}{4\pi\alpha} \vec{b}(t) \vec{e}\right) F(t) &= \int_0^x \frac{u(t)}{\sqrt{x-t}} dt \\ &+ \frac{F(x)}{4\alpha\sqrt{i\pi}} - \frac{1}{8\pi\alpha\sqrt{i\pi}} \int_0^x d\tau F(\tau) \int_\tau^x d\tau \frac{K(t, \tau)}{\sqrt{(x-t)(t-\tau)}}, \end{aligned} \quad (3.25)$$

where

$$K(t, \tau) = \frac{1}{t - \tau} \left\{ \exp \left[\frac{i}{4(t - \tau)} \bar{c}(t, \tau)^2 \right] - 1 \right\}. \quad (3.26)$$

This is again a weakly singular Volterra integral equation which can be discussed and solved by the standard methods. The kernel in the last integral is slightly more complicated than before, this is the price for the simpler structure of the equation. It has recently been proven by Guidotti and Hieber [13] that the integral equation (3.25) has a unique global continuous solution. Numerical calculations are in progress.

Appendix

The inhomogeneous term $u(t)$ in (3.23) comes from

$$u(t) = \frac{\partial}{\partial x} \left(x f_t(\vec{x}) \right) \Big|_{x=0}, \quad (A.1)$$

where $f_t(\vec{x})$ is given by (3.4). The latter quantity is best calculated by Fourier transformation

$$\begin{aligned} f_t(\vec{x}) &= \frac{4\pi N}{(2\pi)^3} \int d^3k \frac{1}{\alpha^2 + k^2} e^{i\vec{k}\vec{x}} \exp \left[-i(\bar{c}(t)\vec{k} + k^2) \right] \\ &= \frac{N}{i\pi} \frac{1}{|\vec{x} - \bar{c}(t)|} A_t(\vec{x}), \end{aligned} \quad (A.2)$$

with

$$A_t(\vec{x}) = \int_{-\infty}^{+\infty} dk \frac{k}{\alpha^2 + k^2} \exp \left[-itk^2 + ik|\vec{x} - \bar{c}| \right]. \quad (A.3)$$

The last integral can be carried out by contour integration

$$A_t(\vec{x}) = \frac{1}{2} \exp \left[\frac{i}{4t} |\vec{x} - \bar{c}|^2 \right] \int_{-\sqrt{it}\infty}^{\sqrt{it}\infty} ds \left(\frac{1}{s - q_1} + \frac{1}{s - q_2} \right) e^{-s^2}. \quad (A.4)$$

Here

$$q_{1,2} = -\sqrt{i} \frac{|\vec{x} - \bar{c}(t)|}{2\sqrt{t}} \pm i\sqrt{it}\alpha \quad (A.5)$$

are the poles in the complex s -plane which lie outside the contour of integration. The last integral (A.4) leads to the complex error function $w(q)$ (2.24) again, so that we finally get

$$u(t) = \frac{N}{2|\bar{c}(t)|} \left[w(q_2) - w(-q_1) \right] \exp \left[\frac{i}{4t} |\bar{c}(t)|^2 \right]. \quad (A.6)$$

References

- [1] S. Geltman, *Journ.Phys.* **B 10**, 831 (1977)
- [2] G. Scharf, K. Sonnenmoser, W.F. Wreszinski, *Phys.Rev* **A 44**, 3250 (1991)
- [3] G. Yao, S. Chu, *Joun.Phys* **B 25**, 363 (1992)
- [4] F.H.M. Faisal, P. Filipowicz, K. Rzazewski, *Phys. Rev.* **A 41**, 6176 (1990)
- [5] P. Deift, E. Trubowitz, *Comm.Pure and Appl.Math* **32**, 121 (1979).
- [6] H.L.Cycon, R.G.Froese, W.Kirsch, B.Simon, *Schrödinger Operators*, Springer Verlag, Berlin 1987, p.140 ff, and references given there.
- [7] D.M.Volkov, *Zeitschr.Phys.* **94**, 250 (1935)
- [8] M.Abramowitz and I.A.Stegun, *Handbook of Mathematical Functions*, Dover Publications
- [9] P.Linz, *Analytical and Numerical Methods for Volterra Equations*, SIAM, Philadelphia 1985
- [10] J. Javanainen, J.H. Eberly, Quichang Su, *Phys.Rev.* **A 38**, 3430 (1988)
- [11] K. Ergenzinger, *Phys.Rev.* **A** to appear
- [12] S.Albeverio, F.Gesztesy, R.Hoegh-Krohn, *Solvable Models in Quantum Mechanics*, Springer 1988
- [13] P.Guidotti, M.Hieber, to appear