# Neutral atom and a charged wire: From elastic scattering to absorption

M. Bawin*
*Université de Liège, Institut de Physique B5, Sart Tilman, 4000 Liège 1, Belgium*

S. A. Coon†
*Physics Department, New Mexico State University, Las Cruces, New Mexico 88003*

(Received 31 May 2000; revised manuscript received 6 September 2000; published 8 February 2001)

We solve the problem of a neutral atom interacting with a charged wire, giving rise to an attractive $1/r^2$ potential in two dimensions. We show how a suitable average over all possible self-adjoint extensions of the radial Schrödinger Hamiltonian eventually leads to the classical formula for absorption of the atom, a formula shown to be in agreement with a recent experiment.

DOI: 10.1103/PhysRevA.63.034701 PACS number(s): 03.75.Be, 02.30.Tb

The scattering of cold neutral atoms by a thin charged wire has, for the first time, allowed the *experimental* study of a pure attractive $1/r^2$ potential in two dimensions [1]. The absorption aspects of this experiment were successfully described by a solution of the classical equations of motion. It is the purpose of this paper to show how this absorption formula can be derived from the *elastic* scattering solutions of the Schrödinger equation for this attractive singular potential [2] instead of introducing *ad hoc* complex phase shifts [3,4]. To do this, we employ a suitable average of the $S$ matrix arising from the mathematically well-defined solutions of the Schrödinger equation with a self-adjoint Hamiltonian and compute the corresponding absorption cross section in the classical limit. Our absorption cross section is then identical to the classical absorption cross section that describes the data of Ref. [1].

To begin, we note that the electrical field of a wire with line charge per unit length $\lambda$ induces a dipole moment $\vec{d}=\alpha\vec{E}$ in a neutral atom of polarizability $\alpha$, which is then attracted towards the wire. The interaction potential in cylindrical coordinates (and Gaussian units so that the fine structure constant $e^2/\hbar c\approx 1/137$),

$$V_{\mathrm{pol}}(r)=-\frac{1}{2}\vec{d}\cdot\vec{E}=-\frac{1}{2}\alpha E^2(r)=-\frac{2\alpha\lambda^2}{r^2}, \tag{1}$$

is always attractive. The radial Schrödinger Hamiltonian for the atom with mass $M$ is

$$H=-\left\{\frac{1}{2M}\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{m^2}{r^2}\right]+\frac{2\alpha\lambda^2}{r^2}\right\}, \tag{2}$$

and the radial Schrödinger equation then becomes

$$\left\{\frac{1}{2M}\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{m^2}{r^2}\right]+\frac{2\alpha\lambda^2}{r^2}+\mathcal{E}\right\}\psi(r)=0, \tag{3}$$

where $m$, the orbital angular momentum quantum number in the $z$ direction (direction of the wire), takes the values $0, \pm 1, \pm 2, \ldots$ and $\mathcal{E}$ is the energy of the atom ($\hbar=c=1$). We require $\nu^2\equiv 4\alpha\lambda^2M-m^2$ to be greater than zero, so that the singular potential remains attractive. We follow Meetz [5] and define a two term regular [6] solution $\phi$ for this singular potential

$$\phi(kr)=C[e^{i\gamma}J_{i\nu}(kr)-e^{-i\gamma}J_{-i\nu}(kr)], \tag{4}$$

with $k^2/2M=\mathcal{E}$, $\nu^2=4\alpha\lambda^2M-m^2$, and $\gamma$ an arbitrary phase, which characterizes the self-adjoint extension [5,7–9] of the radial Schrödinger Hamiltonian (2).

The partial-wave $S$ matrix $S_m$ is given by [10]

$$S_m=\frac{\mathcal{L}_-}{\mathcal{L}_+}, \tag{5}$$

where the Jost function $\mathcal{L}_+$ and $\mathcal{L}_-$ in Eq. (5) are determined by the asymptotic behavior $r\to\infty$ of $\phi(kr)$. This in turn is easily found from [11]:

$$J_\nu(z)\sim\sqrt{\frac{2}{\pi z}}\cos\left(z-\frac{\nu\pi}{2}-\frac{\pi}{4}\right). \tag{6}$$

Comparing Eqs. (4) and (6), we now evaluate the Jost function $\mathcal{L}_+$ and $\mathcal{L}_-$:

$$\phi(kr)\simeq\frac{C}{\sqrt{2kr}}(\mathcal{L}_-e^{ikr}-\mathcal{L}_+e^{-ikr}), \tag{7}$$

and it is not necessary to determine the value of $C$ in Eqs. (4) or (7) as it does not appear in the partial-wave $S$ matrix:

$$S_m(\gamma)=\frac{\mathcal{L}_-}{\mathcal{L}_+}=\frac{e^{i\gamma}e^{\nu\pi/2}-e^{-i\gamma}e^{-\nu\pi/2}}{e^{i\gamma}e^{-\nu\pi/2}-e^{-i\gamma}e^{\nu\pi/2}}. \tag{8}$$

Now we utilize a method suggested by Radin [12] to clarify the relation between the family of solutions in Eq. (4), each solution characterized by $\gamma$ [7], with the alternative unique solution, displaying absorption, found by Nelson [13], for the same attractive $1/r^2$ potential. We, however, apply the method to $S$-matrix elements rather than Radin's

*Email address: michel.bawin@ulg.ac.be
†Email address: coon@nmsu.edu

 

Green functions and we work in two dimensions. Thus, we average $S_m(\gamma)$ over *all* $\gamma$'s corresponding to *all* self-adjoint extensions:

$$\langle S_m \rangle = \frac{1}{2\pi}\int_0^{2\pi} S_m(\gamma)\, d\gamma, \tag{9}$$

and now proceed to show that $\langle S_m \rangle$ displays absorption. Setting $z=e^{i\gamma}$, the average in Eq. (9) becomes

$$2\pi i\langle S_m \rangle = e^{\nu\pi/2}\oint_{|z|=1}\frac{dz}{e^{-\nu\pi/2}z - e^{\nu\pi/2}/z} - e^{-\nu\pi/2}\oint_{|z|=1}\frac{dz/z}{e^{-\nu\pi/2}z^2 - e^{\nu\pi/2}}, \tag{10}$$

and is readily evaluated as

$$\langle S_m \rangle = e^{-\nu\pi}, \tag{11}$$

because the first contour integral of Eq. (10) has no poles inside the contour.

The absorption cross section is given in terms of the partial-wave expansion as [3,14]

$$\sigma_{abs} = \frac{1}{k}\sum_{-\mu}^{+\mu}(1-|S_m|^2). \tag{12}$$

Because $\nu^2 = 4\alpha\lambda^2 M - m^2 > 0$, the limits of the sum on $m$ are given by the integer part of $2\lambda\sqrt{\alpha M}$: $\mu = [2\lambda\sqrt{\alpha M}]$.

In order to take the quantum-mechanical expression (12) to the classical limit, we follow a treatment given by Alliluev [15] in three dimensions. The two-dimensional absorption cross section (12) goes to

$$\sigma_{abs} = \frac{2}{k}\int_0^{+\mu}[1-\exp -2\pi\sqrt{\mu^2-m^2}]dm, \tag{13}$$

where the classical limit is given by $\mu = 2\lambda\sqrt{\alpha M} \gg 1$, see Kayser [16]. The second term in the integral of Eq. (13) is, totally negligible with respect to the first term [one can show the second integral to be $\mathcal{O}(1/\sqrt{\mu})$]. We finally get, from the classical limit of our pure quantum-mechanical treatment of this singular potential

$$\sigma_{abs} = \frac{4\lambda\sqrt{\alpha M}}{k} = 2\sqrt{\frac{4\alpha}{M}\frac{\lambda^2}{v^2}}, \tag{14}$$

where $k = Mv$ and the final form of our result (14) is seen to be identical to Eq. (3) (in the limit of zero radius of the wire) of Ref. [1], obtained by a classical argument.

Now that we have shown how the classical result for absorption by a zero-radius charged wire follows from quantum mechanics, it is straightforward to include classical absorption of an atom with energy $\mathcal{E}$ by the finite radius $R_w$ of the wire by introducing a phenomenological potential of the form $-\beta/r^2$. Classically, those atoms whose impact parameter $\rho$ does not exceed $\rho_{max} = \sqrt{\beta/\mathcal{E}}$ will be absorbed (''fall to the center'') [17]. In two dimensions $\sigma_{abs} = 2\rho_{max}$. For the uncharged wire of radius $R_w$ one gets $\sigma_{abs} = 2R_w$ for a phenomenological strength $\beta = R_w^2\mathcal{E}$. With $\beta = R_w^2\mathcal{E} + 2\alpha\lambda^2$, it is clear that classically one has

$$\sigma_{abs} = 2\sqrt{R_w^2 + \frac{4\alpha}{M}\frac{\lambda^2}{v^2}} \tag{15}$$

in agreement with Eq. (15) in Ref. [1]. Note that the phenomenological classical potential we adopt for the uncharged wire with a finite radius is also singular, a choice ultimately justified by the successful description of the data by Eq. (15) in Ref. [1].

We have emphasized the rigorous mathematics of this problem to illustrate the point that there is no difficulty, neither quantum mechanically nor mathematically, with formulating the problem of the interaction of a polarizable atom with a zero-radius line charge, contrary to statements in the physics literature [18]. Attempts have been made to give the continuous parameter $\gamma$ of the self-adjoint extensions of the radial Schroedinger Hamiltonian with an attractive $1/r^2$ potential a physical interpretation [9,19]. One such interpretation is briefly discussed in the appendix in conjunction with a different method of solving Eq. (3). However, given the difficulty in trying to select a unique self-adjoint extension based upon physical arguments [9], we instead have shown that, by considering *all* self-adjoint extensions by averaging over $\gamma$, one can go from a well-formulated quantum-mechanical elastic-scattering solution to the classical formula for absorption, a formula which fits the experimental data.

The work of M.B. was supported by the National Fund for Scientific Research, Belgium and that of S.A.C. by NSF Grant No. PHY-9722122.

## APPENDIX

For completeness sake, we briefly discuss how the quantum-mechanical expression (11) can be derived from the approach of the authors of Ref. [9]. These authors write the physical solution [6] $R_m(kr)$ to Eq. (3) as

$$R_m(kr) = a_m J_{-\nu}(kr) + b_m J_\nu(kr), \tag{A1}$$

where $a_m$ and $b_m$ are determined by requiring the radial wave functions to form an orthogonal set. They then find $R_m(kr)$ to be of the form

$$R_m(kr) = c_m[\exp i[\theta_m + 2\mu\ln(k/M)]J_{-i\nu}(kr) + J_{i\nu}(kr)], \tag{A2}$$

where $c_m$ is a normalization factor and $\theta_m$ a phase characterizing the self-adjoint extension. From Eqs. (A2) and (6) one now finds the partial-wave $\tilde{S}_m$ to be given by

$$\tilde{S}_m = \frac{\exp i(\theta_m + 2\nu\log k/M)e^{-\nu\pi/2} + e^{\nu\pi/2}}{\exp i(\theta_m + 2\nu\log k/M)e^{\nu\pi/2} + e^{-\nu\pi/2}}, \tag{A3}$$

since the connection between $\tilde{S}_m$ and the asymptotic form of $R_m(kr)$ is [9]

$$R_m(\rho) \to \sqrt{\frac{1}{2\pi p\rho}}[\exp -i(p\rho - \pi m - \pi/4) + \tilde{S}_m \exp i(p\rho - \pi/4)]. \quad \text{(A4)}$$

From Eq. (A3), one then finds the poles of $\tilde{S}_m$ (bound states) to be of the form $k = i\kappa$, with

$$\kappa = \exp \theta'_m - 2\pi n/2\nu, \quad n = 0, \pm 1, \pm 2, \ldots, \quad \text{(A5)}$$

and

$$\theta'_m = \pi - \theta_m . \quad \text{(A6)}$$

Equation (A5) shows that the domain of $\theta'_m$ is

$$0 \leqslant \theta'_m < 2\pi, \quad \text{(A7)}$$

in order to include all possible values of $\kappa$ in Radin's sum over *all* possible self-adjoint extensions. Taking Eq. (A6) into account one can then compute $\langle \tilde{S}_m \rangle$ in Eq. (A3) exactly as before and obtain again our result (11) by introducing now the variable $z = e^{i\theta'_m}$. Thus, the ''pragmatic'' approach of the authors of Ref. [9] yields exactly the same average partial-wave $S$ matrix as does our approach based upon a straightforward application of mathematically rigorous but perhaps less familiar techniques. Indeed, from Eq. (A5), one can see that choosing one specific self-adjoint extension amounts to making the bound-states spectrum unique by specifying the position of *one* level in the spectrum [19]. We thus have demonstrated, with the elastic-scattering solutions of Ref. [9], that our averaging procedure leading to absorption and ultimately to the correct classical limit can be viewed as an average over all ways of specifying a unique quantum-mechanical bound-state spectrum.


[1] J. Denschlag, G. Umshaus, and J. Schmiedmayer, Phys. Rev. Lett. **81**, 737 (1998).

[2] By definition, a cylindrically symmetrical singular potential $V(r)$ is characterized by the property $\lim_{r\to 0}[r^2 V(r)] \neq 0$. For an attractive singular potential the possibility, classically, that the particle ''fall'' into the potential hole (Ref. [3]) corresponds, in the quantized theory, to an ambiguity in the choice of the radial wave function, which implies the impossibility to obtain unambiguously the scattering phase shift. The mathematical characterization of this ambiguity lies in the statement that ''singular differential operators are either self-adjoint or give rise to a well-defined class of self-adjoint extensions in the Hilbert space of square-integrable functions $L_2(0,\infty)$,'' taken from Ref. [5].

[3] J. Denschlag and J. Schmiedmayer, Europhys. Lett. **38**, 405 (1997).

[4] J. Audretsch and V. D. Skarzhinsky, Phys. Rev. A **60**, 1854 (1999).

[5] K. Meetz, Nuovo Cimento **34**, 690 (1964).

[6] The regular solution is defined by boundary conditions *at a single point*, in this case the point $r=0$, rather than the physical solution defined by mixed boundary condition, one at $r=0$ and one at $r=\infty$. See for example, Ref. [10].

[7] K. M. Case, Phys. Rev. **80**, 797 (1950).

[8] W. G. Faris, *Self-Adjoint Operators*, Lecture Notes in Mathematics Vol. 433 (Springer, Berlin, 1975).

[9] J. Audretsch, V. D. Skarzhinsky, and B. L. Voronov, quant-ph/0004065 (unpublished).

[10] R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), Chap. 12.

[11] *Handbook of Mathematical Functions*, edited by M. Abramovitz and I. A. Stegun (Dover, New York, 1967), p. 364.

[12] C. Radin, J. Math. Phys. **16**, 544 (1975).

[13] E. Nelson, J. Math. Phys. **5**, 332 (1964).

[14] K. Gottfried, *Quantum Mechanics* (Benjamin, New York, 1966), pp. 127–129. The analogous formulas for two dimensions are derived by I. R. Lapidus, Am. J. Phys. **50**, 45 (1982); **54**, 459 (1986).

[15] S. P. Alliluev, Zh. Éksp. Teor. Fiz. **61**, 15 (1971) [Sov. Phys. JETP **34**, 8 (1972)].

[16] B. Kayser, Am. J. Phys. **42**, 960 (1974). This paper demonstrates clearly that quantum-mechanical scattering from a $1/r^2$ potential becomes classical only when the potential is *strong*, the condition of the experiment of Ref. [1].

[17] L. D. Landau and E. M. Lifshitz, *Mechanics* (Pergamon, London, 1960), p. 51.

[18] C. R. Hagen, Phys. Rev. Lett. **77**, 1656 (1996).

[19] A. M. Perelomov and V. S. Popov, Teor. Mat. Fiz. **4**, 48 (1970) [Theor. Math. Phys. **4**, 664 (1970)].