Fitting scenarios in a simple theoretical approach to 1s level shifts in pionic atoms

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The Klein-Gordon version of a simple analytic model of the pionic atom due to M. Ericson is derived. The expected precision of the resulting expression for pionic atom 1s level shifts is about 10%. The model is well-suited for the qualitative comparison of theory, especially with regard to various parametric fitting strategies, and experiment in this case. It is found that a repulsive ReB_0 , comparable with $\text{Im}B_0$ in magnitude, is required to fit the experimental (T=0) data in the low A region.

I. INTRODUCTION

The set of parameters which characterizes the complex pion-nucleus optical potential derived from the multiple scattering theory some time ago by Ericson and Ericson¹ continues to be a useful basis for describing fits to experimental data on level shifts (ΔE) [and widths (Γ)] of pionic atoms. Lately, in keeping with the increasing accuracy of the experimental data, the theoretical predictions of ΔE and Γ of Krell and Ericson² from this optical potential,³

$$2\overline{m}_{\pi}V_{\text{opt}} = q(r) - \nabla \cdot \alpha(r) \nabla , \qquad (1)$$

$$q(r) = 4\pi \{ p_1 b_0 \rho(r) + p_1 b_1 [\rho_n(r) - \rho_p(r)] + p_2 B_0 \rho^2(r) \},$$
(2)

$$\alpha(r) = \alpha_0(r) / [1 - \xi \alpha_0(r) / 3], \qquad (3)$$

$$\alpha_{0}(r) = -4\pi \{ p_{1}^{-1} c_{0} \rho(r) + p_{1}^{-1} c_{1} [\rho_{n}(r) - \rho_{p}(r)] + p_{2}^{-1} C_{0} \rho^{2}(r) \}$$
(4)

have entailed numerical solution of the bound-state Klein-Gordon equation,⁴

$$\{\nabla^{2} + [(E - V_{C})^{2} - \overline{m}_{\pi}^{2}]\}\psi = 2\overline{m}_{\pi}V_{\text{opt}}\psi; \qquad (5)$$

this is customarily accomplished by transforming the resulting nonlocal radial Schrödinger equation,

$$\{-p_r^2 + l(l+1)/r^2 + [(E_{nl} - V_C)^2 - \overline{m}_{\pi}^2]\}(u_{nl}/r) = [q(u_{nl}/r) - \alpha'(r)d(u_{nl}/r)/dr] - \alpha[-p_r^2 + l(l+1)/r^2](u_{nl}/r), \quad (6)$$

$$w_{nl}'' - [l(l+1)/r^{2}]w_{nl} + [(E_{nl} - V_{C})^{2} - \overline{m}_{\pi}^{2}]w_{nl}/[1 + \alpha(r)] = \{q(r) + \alpha'(r)/r - [\alpha'(r)/2]^{2}/[1 + \alpha(r)] + (\frac{1}{2})\alpha''(r)\}w_{nl}/[1 + \alpha(r)], \quad (7)$$

by means of the factorization,

$$u_{nl} = (1+\alpha)^{-1/2} w_{nl} \ . \tag{8}$$

However, prior to this technical development, for a qualitative comparison with the experimental data, one might have turned to the model introduced by M. Ericson^{1,6} which yields pionic atom energy shifts (and widths) expressed both analytically and simply. Specifically the complex energy shifts are given there by an expansion whose precision "has been estimated to be of the order of 10% for the 1s level shifts in ¹⁶O and ¹⁹F."¹ Although the accuracy⁷ of the 1s experimental data has improved in the meanwhile, such a model is still quite suitable for a qualitative comparison between theory, especially in regard to conventionally accepted fitting scenarios,

and experiment. It should be added that the relatively crude treatment of the nuclear surface in this model (see Sec. II below and Refs. 1 and 6) is of less moment for the 1s level shifts; these, being negative, reflect the dominant role played by the real part of the "local part" of $2\overline{m}_{\pi}V_{\text{opt}}$, q(r), in this case.

In Sec. II, the more appropriate Klein-Gordon (rather than the original Schrödinger^{1,6}) version of this model is derived. (The expression for the Schrödinger version of the shift which appears in Refs. 1 and 8, later quoted verbatim in Kim's monograph on mesic atoms,⁹ contains some troublesome misprints.) Section III is concerned mainly with the qualitative comparison of two conventionally accepted fitting scenarios; it is easy to include in this comparison a parameter set representative of a model of strong *P*-wave medium polarization.¹⁰

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Nuclear parameters^a $\operatorname{Re}\Delta E(1s;\operatorname{strong})/Z^4$ R С Ζ W Approximation (Klein-Gordon version) Exact (eV) (fm) (fm)(fm) (fm) (eV) 1.008 0.327 0.445 ⁴₂He -5.712 -6.807 2.21 ²⁰Ne ²⁴Ng 3.87 0.569 -4.096 2.74 -3.8542.99 0.548 -3.7223.98 -3.600

TABLE I. Comparison of approximate (Klein-Gordon version) and exact theoretical calculations of the reduced strong-interaction 1s level shift in selected nuclei.

*These are taken from Ref. 20.

II. THE MODEL

It simplifies matters if we begin with the original formulation which deals with a bound nonrelativistic pion moving in accordance with the Schrödinger equation. One takes for the nucleus a square well with radius Requal to the equivalent mean square radius obtained in electron scattering analyses; thus, $R = (\frac{5}{3})^{1/2} \langle r^2 \rangle^{1/2}$. The Coulomb potential is given by

$$V_{C} = -(3Z\alpha/2R)[1-(\frac{1}{3})(r/R)^{2}], (r < R)$$

= -(Z\alpha/r), (r > R) (9)

with $\rho(r) = A/(4\pi^3/3)\theta(R-r)$ determining the behavior of $V_{\text{opt}}(r)$.

In the case of perturbed 1s states, one has to deal with the Schrödinger equation,

$$H\psi_1 = (E_1 + \Delta E)\psi_1 , \qquad (10)$$

where

$$E_1 = -\overline{m}_{\pi} (Z\alpha)^2 / 2 \tag{11}$$

is the unperturbed energy in the absence of both finite size Coulomb and nuclear effects which are contained in ΔE . *H* is given by¹¹

$$H = -(\nabla^2 / 2\bar{m}_{\pi}) + (-4\pi / 2\bar{m}_{\pi})(b_0 \rho_0 \theta(R - r) - \nabla \cdot \{c_0 \rho_0 \theta(R - r) / [1 + (4\pi / 3)\xi c_0 \rho_0]\} \nabla) + \theta(R - r)(Z\alpha / 2R)[-3 + (r/R)^2] + \theta(r - R)(-Z\alpha / r) ,$$
(12)

where

$$\rho_0 = A / (4\pi R^3 / 3) ; \tag{13}$$

let us assume for the moment that N = Z. The integration over an infinitesimal shell about the nuclear surface at r = R yields the relation between radial derivatives of the inside (-) and outside (+) radial solutions:

$$-(d\psi_{1+}/dr)_R + (1+A)(d\psi_{1-}/dr)_R = 0, \qquad (14)$$

with

$$A = -4\pi \{ c_0 \rho_0 / [1 + (4\pi/3)\xi c_0 \rho_0] \} .$$
⁽¹⁵⁾

After introducing the dimensionless variables,^{12,13}

$$x = [-8\overline{m}_{\pi}(E_1 + \Delta E)]^{1/2} r \equiv 2kr , \qquad (16)$$

$$\xi = (Z \alpha \overline{m}_{\rm eff} / R^3)^{1/4} r \equiv \beta^{1/2} r , \qquad (17)$$

we easily produce the outside and inside radial equations for the radial wave function, $u_1 = r\psi_1$. In the outside region, u_1 is a Whittaker function,¹⁴ $W_{\kappa,1/2}(x)$, given asymptotically by

$$u_1 \sim e^{-x/2} x^{\kappa-1} [1 - \kappa(\kappa-1)/x];$$
 (18)

in the inside region, u_1 is a confluent hypergeometric function¹⁵ of ξ^2 , with

$$u \sim e^{-\xi^2/2} \xi M(\frac{3}{4} - K^2/4\beta | \frac{3}{2} | \xi^2) , \qquad (19)$$

where

$$K^{2} = 2\overline{m}_{\rm eff}(E_{1} + \Delta E) + 3Z\alpha\overline{m}_{\rm eff}/R + 4\pi b_{0}\rho_{0}/(1+A)$$
(20)

TABLE II. Experimental strong-interaction 1s level shift data selected for comparison with theory.

⁴ ZElement	1s level shift (keV)	Reference
⁴ ₂ He	-0.079 ± 0.005	21
3Li	-0.324 ± 0.003	22
3 ¹ Li	-0.570 ± 0.004	22
åBe	-1.595 ± 0.009	22
¹⁰ 5 B	-2.977 ± 0.085^{a}	23
¹¹ 5 B	-3.839±0.085ª	23
¹² ₆ C	-5.874±0.092ª	23
¹⁴ 7N	-9.915±0.144ª	23
¹⁶ ₈ O	-15.64 ± 0.10	24
¹⁸ ₈ O	-20.21 ± 0.10	24
¹ % F	-25.68 ± 0.16	25
²⁰ ₁₀ Ne	-33.34 ± 0.50	23
²³ ₁₁ Na	-51.40 ± 0.27	25
$^{nat}_{12}Mg$	-57.1 ± 1.4	26

^aThese experimental data are taken from averaged values provided by Tauscher and Schneider (Ref. 23).

TABLE III. Some characteristic parameter sets (1970-1985).

	$b_0(m^{-1})$	$b_1(m^{-1})$	$c_0(m^{-3})$	$c_1(m^{-3})$	$B_0(m^{-4})$	$C_0(m^{-6})$
$ \frac{1}{Backenstoss^{a}} $ $ (\xi = 1.0) $	-0.03	-0.087	0.21	0.18	(0.0,0.017)	(0.0,0.073)
Tauscher ^b $(\xi = 1.0)$	-0.0293	-0.078	0.227	0.18	(0.0,0.0428)	(0.0,0.076)
Batty et al. ^c $(\xi=1.0)$	-0.017	-0.13	0.255	0.17	(-0.0475,0.0475)	(0.0,0.90)
Batty et al. ^d $(\xi = 1, 0)$	-0.017	-0.12	0.21	0.17	(-0.0475,0.0475)	(0.0829,0.0425)
Stricker <i>et al.</i> ^e $(\xi=0.6)$	-0.032	-0.078	0.24	0.22	(-0.043,0.023)	(-0.1,0.1)
Stricker <i>et al.</i> ^f $(\xi = 1, 4)$	-0.0325	-0.095	0.234	0.151	(-0.002,0.048)	(0.036,0.116)
Poffenberger ^g $(\xi = 1.0)$	-0.0291	-0.0839	0.246	0.0	(0.0,0.0433)	(0.0,0.101)
Poffenberger ^h $(\xi = 1.0)$	-0.0177	-0.0939	0.241	0.0	(-0.0501,0.0443)	(0.0,0.112)
<i>P</i> -wave medium polarization ⁱ $(\xi = 1.0)$	-0.0513	-0.097	0.246	0.0	(0.0,0.0433)	(0.0,0.101)

^aReference 27.

^bReference 28.

^cReference 19.

^dReference 31.

eReference 33.

^fReference 29.

^gReference 30.

^hReference 30.

ⁱReference 10.

The matching condition between ψ_{1-} and ψ_{1+} implied by Eq. (14) simplifies to

$$\left[-(\frac{1}{3})K^{2}R^{2}+(\frac{1}{5})\beta^{2}R^{4}-(\frac{1}{45})K^{4}R^{4}\right](1+A)$$

=-kR+(\kappa-1)+R\kappa(\kappa-1)/2kR^{2}, (21)

after expanding "inside" quantities in powers of R^2 . Introducing

$$k_1 = Z \alpha \overline{m}_{\pi} , \qquad (22)$$

and substituting the first-order expansions,

$$\kappa - 1 \simeq - \left(\frac{1}{2}\right) \left(\Delta E / E_1\right) , \qquad (23)$$

$$k \simeq k_1 (1 + \Delta E / 2E_1) , \qquad (24)$$

into Eq. (21), one obtains the Schrödinger version of the 1s level shift formula:

$$(\Delta E/E_1)(1+2k_1R+2k_1^2R^2) = -4k_1^2R^2 - 4k_1R\{k_1R/[5(1+A)] - K^2R^2/3 + 3k_1K^2R^3/[20(1+A)] - K^4R^4/45\}(1+A),$$
(25)

with¹⁶

.

$$K^{2}R^{2} = \left(-k_{1}^{2}R^{2} + 4\pi\rho_{0}b_{0}R^{2} + 3k_{1}R\right)/(1+A) . \quad (26)$$

[We must point out that while the Klein-Gordon corrections to this result, Eq. (25), prove to be inconsiderable for the range of Z values which concern us in this paper, our result still differs from that of Refs. 1, 6, and 9 in the R^2 term in the coefficient of $\Delta E/E_1$ on the left-hand side of Eq. (25).]

The same asymptotic expansion as before suffices for the outside solution in the Klein-Gordon version. Now one finds

$$\kappa - 1 \simeq -(\frac{3}{8})Z^2 \alpha^2 - (\frac{1}{2})(\Delta E/E_1)$$
, (27)

$$k \simeq k_1 [1 - (Z^2 \alpha^2 / 8) + (\frac{1}{2})(\Delta E / E_1)],$$
 (28)

at the same time, with the neglect of a small anharmonicity $[O(r^4)$ in the $V_C^2]$ contribution to the effective inside potential, the inside solution satisfies a differential equation of the same form as before. Thus, relativity introduces modifications in the Schrödinger result [Eq. (25)] $O(Z^2\alpha^2)$ which take the form of a substitution rule on it:



FIG. 1. Predictions of the simple Klein-Gordon approach to 1s level shifts for nuclei with isospin T=0, $\frac{1}{2}$, and 1 are given by the uppermost, central, and lowest curves using the parameter set of Backenstoss (Ref. 27) (see Table III) with input nuclear rms radii taken from Table IV. The experimental points $[O's (\times's)$ denote T=0 ($\frac{1}{2}$) nuclei, the \Box denotes the T=1 nucleus ${}^{16}O$] with associated error bars are taken from Table II [fitting scenario (a)].

TABLE IV. Nuclear rms radii (taken from Ref. 20) input for the solid curves of Figs. 1–9. The extensions of the plots required the additional input from the nuclei, 27 Al, 28 Si, 31 P, and 32 S, with rms (in fm) 3.05, 3.10, 3.187, and 3.238, respectively (Ref. 20).

	$\langle r^2 \rangle^{1/2}$	
$^{A}_{Z}$ Element	(fm)	
⁴ ₂ He	1.71	
3Li	2.57	
3 L i	2.41	
⁹ Be	2.51	
¹⁰ 5B	2.45	
¹¹ ₅ B	2.37	
¹² ₆ C	2.46	
¹⁴ 7N	2.54	
¹⁶ / ₈ O	2.674	
¹⁸ 80	2.76	
¹ 9F	2.85	
²⁰ Ne	2.80	
²³ ₁₁ Na	2.94	
²⁴ ₁₂ Mg	3.08	

$$[\text{rhs of Eq. (26)}] \rightarrow -4k_1 R \{k_1 R (1 - Z^2 \alpha^2 / 8) + (\frac{3}{8}) Z^2 \alpha^2 - (\frac{5}{16}) (Z^2 \alpha^2 / k_1 R) + (1 + A) [-(\frac{1}{3}) K_{\text{rel}}^2 R^2 + (\frac{1}{5}) \beta_{\text{rel}}^2 R^4 - (\frac{1}{45}) K_{\text{rel}}^4 R^4 + (\frac{3}{20}) \beta_{\text{rel}}^2 K_{\text{rel}}^2 R^6]\}, \qquad (29)$$

with

$$K_{\rm rel}^2 R^2 = [-k_1^2 R^2 + 4\pi \rho_0 b_0 R^3 + 3k_1 R + (\frac{9}{4}) Z^2 \alpha^2] / (1+A) , \qquad (30)$$

$$\beta_{\rm rel}^2 R^4 = [k_1 R + (\frac{3}{2}) Z^2 \alpha^2] / (1+A) . \tag{31}$$

To obtain some idea of the precision of the Klein-Gordon expansion [Eqs. (26), (29), (30), and (31)], we have compared its predictions for $\text{Re}\Delta E(1s;\text{strong})$ (Ref. 17)



FIG. 2. The same as Fig. 1 but with the parameter set of Ref. 28 (see also Ref. 23). Fitting scenario (a).

with those of an exact calculation¹⁸ which uses the local form of the effective potential [Eq. (7)] in three cases, ${}_{2}^{4}$ He, ${}_{10}^{20}$ Ne, and ${}_{12}^{24}$ Mg, using a parameter set of Batty et al.¹⁹ (See Table I, where the parameters characterizing the different nuclear Fermi shapes²⁰ are given.) It is convenient (see Sec. III below) to work with reduced 1s level shifts, Re $\Delta E(1s;$ strong)/Z⁴. One sees in these cases that the estimate of the precision of the approximate approach as given in Ref. 1 is quite reasonable.



FIG. 3. The same as Fig. 1 but with the parameter set of Ref. 19. Fitting scenario (b).



FIG. 4. The same as Fig. 1 but with the parameter set of Ref. 31. Fitting scenario (b).

III. FITTING SCENARIOS AND THE COMPARISON WITH THE DATA

It is readily seen that in spite of the 10% margin of precision which characterizes the approximate result obtained above [Eqs. (26), (29), (30), and (31)], such a theory is nevertheless well suited for making qualitative judgments of the way in which various fitting strategies have accommodated to the experimental 1s level shift data over the past fifteen years. The data referred to in this study (see Table II) include all of the highly accurate data (with accuracies ~1%) obtained within the last decade or so: ⁴He (Ref. 21); ⁶Li, ⁷Li, and ⁹Be (Ref. 22); ¹⁰B, ¹¹B, ¹²C, ¹⁴N, and ²⁰Ne (Ref. 23); ¹⁶O and ¹⁸O (Ref. 24); ¹⁹F and ²³Na (Ref. 25); and ^{nat}Mg (Ref. 26).

For our survey we have assembled nine typical parameter sets (see Table III) used with varying degrees of success from 1970 to 1985. It should be pointed out that these parameter values are also dependent somewhat on the values taken for the nuclear rms radii, and the latter, we note, have in a number of cases inflated over this same period. In spite of this additional source of uncertainty



FIG. 5. The same as Fig. 1 but with the parameter set of Ref. 33. The fit here is less than satisfactory. Fitting scenario (b).



FIG. 6. The same as Fig. 1 but with the parameter set of Ref. 29. Fitting scenario (a).

(which does not seem to get in the way of the ability of the approximate approach to distinguish between "good" and "bad" fits to the data), to make life simpler we have uniformly used entries from the 1974 compilation of de Jager et al.²⁰ (see the tabulation of rms radii in Table IV) in the calculations reported here. Furthermore it is useful to make the comparison of the data with the fits for $T=0, \frac{1}{2}$, and 1 nuclei in terms of "reduced" level shifts.^{22,27} Re $\Delta E(1s; strong)/Z^4$. One distinguishes two classes of fit, scenario (a), characterized by $\text{Re}B_0 = 0$, and scenario (b), characterized by $\text{Re}B_0 = -\text{Im}B_0$ (i.e., $\text{Re}B_0$ sizable and repulsive). The fits of Figs. 1, 2, 6, and 7 which were made in the period 1970-1981 typify good fits^{27-30,32} according to scenario (a). Note that the trend of the data for A > 10 is well represented while there is no possibility of fitting the sharp divergence from the overall smooth behavior at A=6. The fits of Figs. 3, 4, and 8 which were made in the period 1978-1981 typify good fits^{19,30,31} according to scenario (b). Note that fits according to scenario (b) fit both the overall smooth behavior



FIG. 7. The same as Fig. 1 but with a parameter set of Ref. 30. Fitting scenario (a).



FIG. 8. The same as Fig. 1 but with a parameter set of Ref. 30. Fitting scenario (b).

with A as well as the "kink" at A=6. Aside from the phenomenological necessity for $\text{Re}B_0 = -\text{Im}B_0$, which implies a sizable (real) repulsive ρ^2 strength in the lowenergy pion-nucleus optical potential, one infers that ⁶Li has a more diffuse structure than its neighbors, ⁴He and ¹⁰B. It should be pointed out that our approach can distinguish fits to the 1s data that are less than satisfactory, e.g., the fit³³ exhibited in Fig. 5 according to scenario (b). It is interesting to comment on the rather poor fit provided by a parameter set representative of a model of strong *P*-wave medium polarization in the present context (see Fig. 9). This is doubtless a consequence of an excessively large value of $|b_0|$. This is noted in the first citation of



FIG. 9. The same as Fig. 1 but with the parameter set relevant to a model (Ref. 10) of *P*-wave medium polarization. The fit to the data here is very poor. Fitting scenario (a).

Ref. 10. However, the remedy, suggested there,¹⁰ of utilizing a possible source of ρ^2 attraction (Re $B_0 \ge 0$), will undoubtedly exacerbate the divergence between fit and data around A=6 which is already obtained in this model. We should like to suggest that this situation may be improved somewhat by the accommodation in this theory of particle-hole contributions. (We remark that this poor showing is insensitive to the changes in the values of the ξ parameter.)

This work was supported in part by the Rutgers Research Council.

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- ${}^{4}V_{c}$ is the Coulomb potential for the extended nuclear charge and E is the pion eigenenergy which includes the pion rest mass m_{π} ($\hbar = c = 1$).
- ⁵Note that we have taken the liberty of correcting a bothersome misprint in Eq. (5) of Ref. 2.
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effects of pion absorption in the following derivation.

- ${}^{12}\widetilde{E} \equiv E_1 + \Delta E \text{ and } \overline{m}_{\text{eff}} = \overline{m}_{\pi} / (1+A).$
- ¹³We also write $\kappa = \overline{m}_{\pi} Z \alpha / k$.
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- ¹⁶For nuclei with $N \neq Z$, the additional substitution, $(b_0, c_0) \rightarrow (b_0, c_0) + (b_1, c_1)(N - Z)/A$, should be made. (This is aside from the additional substitutions relating to absorption.)
- ¹⁷This is the 1*s* level shift due to the strong interaction alone.
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