Chiral Dynamics of Deeply Bound Pionic Atoms

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We present and discuss a systematic calculation, based on two-loop chiral perturbation theory, of the pion-nuclear s-wave optical potential. A proper treatment of the explicit energy dependence of the off-shell pion self-energy together with (electromagnetic) gauge invariance of the Klein-Gordon equation turns out to be crucial. Accurate data for the binding energies and widths of the 1s and 2p levels in pionic ²⁰⁵Pb and ²⁰⁷Pb are well reproduced without need for a notorious “missing repulsion” in the pion-nuclear s-wave optical potential. The connection with the in-medium change of the pion decay constant is clarified.

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Recent accurate data on 1s and 2p states of negatively charged pions bound to Pb nuclei [1] have set new standards and constraints for the detailed analysis of s-wave pion-nucleus interactions. This subject has a long history [2–8], culminating in various attempts to understand the notorious missing repulsion: The standard ansatz for the s-wave pion-nucleus optical potential in terms of the empirical threshold πN amplitudes times the proton and neutron densities ρ_p,n, supplemented by sizable double-scattering corrections, still misses the empirically required repulsive interaction by a large amount. On purely phenomenological grounds, this problem can be fixed by simply introducing a sufficiently large negative real part, Re B_0, in the ρ^2 term of the pion-nuclear potential [6]. The arbitrariness of this procedure is of course unsatisfactory, also in view of the fact that Re B_0 cannot be calculated microscopically with sufficient accuracy, and that the high precision measurements of the real part of the pion deuteron scattering length [9] suggests a very small net Re B_0 by analogy.

In the meantime, this issue has been revived in a variety of ways. An interpretation of the missing repulsion in terms of a possible in-medium change of the pion decay constant, as suggested in Ref. [10], appears to be remarkably successful [11,12] but has been debated [13,14]. Clearly, this concept needs further justification.

In the present paper, we show that a possible key to the understanding of low-energy pion-nucleus interactions lies in its distinct energy dependence imposed by chiral symmetry, in combination with the “accidental” approximate vanishing of the isospin-even threshold πN amplitude [15]. Another important feature, generally ignored in previous analyses, is the systematic incorporation of gauge invariance at all places where the pion energy ω appears explicitly, when solving the Klein-Gordon equation in the presence of electromagnetic interactions.

Our framework will be in-medium chiral perturbation theory at two-loop order [16]. But before going into technical details, the following simplified treatment may be useful to illustrate driving mechanisms.

Consider a zero-momentum π^- interacting with nuclear matter at low proton and neutron densities, ρ_p and ρ_n. The in-medium pion polarization operator to leading order in the nucleon densities is expressed in terms of the isospin-even and isospin-odd off-shell πN amplitudes T_+ (ω) as Π(ω) = - T_+ (ω) δρ - T_+ (ω) ρ, with the isoscalar and isovector nucleon densities, ρ = ρ_p + ρ_n and δρ = ρ_p - ρ_n. The spontaneous and explicit breaking of chiral symmetry implies the following leading terms of those amplitudes [17]:

\[ T_+ (ω) = \frac{σ_N - βω^2}{f_π^2}, \quad T_- (ω) = \frac{ω}{2f_π^2}, \]

where f_π = 92.4 MeV is the pion decay constant, m_π = 139.57 MeV is the (charged) pion mass, and σ_N ≈ 45 ± 8 MeV [18] is the pion-nucleon sigma term. The empirical observation that T_+ (m_π) = (-0.04 ± 0.09) fm ≈ 0 [19] sets the constraint β ≈ σ_N/m_π.

Next, consider the pionic in-medium dispersion equation at zero momentum, ω_0^2 - m_π^2 = Π(ω) = 0. Introduce an (energy independent) equivalent optical potential U by ω_0^2 - m_π^2 = m_π^2 + 2m_π U with U ≪ m_π, and expand around ω = m_π. This gives

\[ U \approx \frac{Π(m_π)}{2m_π} \left[ 1 + \frac{Π(m_π)}{2m_π} \right] + \cdots \approx \frac{Π(m_π)}{2m_π} (1 - \frac{1}{2Π}) \frac{1}{ω = m_π}, \]

where the last approximate step introduces the wave function renormalization factor \{1 - (dΠ)/(dω^2)\}_ω=m_π^{-1}. The difference between the second and the last step in (2) is of subleading order. Inserting (1) and assuming δρ ≪ ρ, one finds

\[ U \approx - \frac{δρ}{4f_π^2} \left( 1 - \frac{σ_N ρ}{m_π^2 f_π^2} \right) \approx - \frac{δρ}{4f_π^2}, \]

which is the expression proposed in Ref. [10]. It involves the driving Weinberg-Tomozawa term in T_- (ω), but with the pion decay constant renormalized [f_π → f_π(ρ)] to

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leading order in the density $\rho_0$ in accordance with the corresponding in-medium change of the chiral quark condensate $\langle \bar{q}q \rangle$.

To the extent that $U$ represents part of the (energy independent) s-wave optical potential commonly used in the phenomenological analysis of pionic atoms, at least part of the missing repulsion is thus given a physical interpretation in terms of the reduced in-medium $f_\pi$ in the denominator of (3). Of course, rather than constructing the potential $U$ and following the steps leading to (2) and (3), one can directly solve the Klein-Gordon (KG) equation with the full energy dependence of the polarization operator $\Pi(\omega)$. This is the procedure systematically applied in this paper, with proper recognition of gauge invariance in the presence of the electromagnetic field.

The KG equation with Coulomb potential $V_c(\vec{r}) < 0$ and total pion self-energy, $\Pi_{\text{tot}}(\omega, \vec{r})$, reads

$$[(\omega - V_c)^2 + \nabla^2 - m_\pi^2 - \Pi_{\text{tot}}(\omega, V_c, \vec{r})] \Phi(\vec{r}) = 0.$$

(4)

The total polarization operator expressed in terms of local proton and neutron densities, $\Pi_{\text{tot}}(\omega, \vec{r}) = \Pi_{\text{tot}}(\omega; \rho_p(\vec{r}), \rho_n(\vec{r}))$, can be split into its s-wave and p-wave parts:

$$\Pi_{\text{tot}}(\omega; \rho_p, \rho_n) = \Pi(\omega) + \Delta \Pi_S(\omega; \rho_p, \rho_n)$$

$$+ \Pi_P(\omega; \rho_p, \rho_n),$$

where we separate explicitly the phenomenological s-wave absorption term quadratic in densities,

$$\Delta \Pi_S(\omega; \rho_p, \rho_n) = -8\pi \left(1 + \frac{m_\pi}{2M}\right) B_0 \rho_p(\rho_n + p_p).$$

(5)

parametrized as in Ref. [6]. Here $M$ stands for the nucleon mass. We use $\text{Im} B_0 = 0.063 m_\pi^{-4}$ from Ref. [4] and $\text{Re} B_0 = 0$ as our standard set and discuss variations of the $\text{Re} B_0$ and $\text{Im} B_0$ later. For the p-wave part $\Pi_P(\omega; \rho_p, \rho_n)$, we use the traditional Kisslinger form with inclusion of short-range correlations and parameters as specified in Ref. [4] (set A). The regular s-wave part, $\Pi(\omega)$, will be in the center of our consideration below.

Given the smallness of the isospin-even $\pi N$ scattering amplitude $T^+(\omega)$, double-scattering (Pauli-blocking) corrections in $\Pi(\omega)$ are well known to be important [2]. When those are included, the “phenomenological” s-wave pion polarization operator becomes [7]

$$\Pi_{\text{phen}}(\omega; \rho_p, \rho_n) = -T^-(\omega) \delta \rho - T^+_{\text{eff}}(\omega, \rho) \rho,$$

(6)

with

$$T^+_{\text{eff}}(\omega, \rho) = T^+(\omega) - \frac{3k_F}{8\pi^2} \left[\langle T^+(\omega) \rangle^2 + 2\langle T^-(\omega) \rangle^2\right].$$

(7)

The local Fermi momentum $k_F(r) = [3\pi^2 \rho(r)/2]^{1/3}$ is rewritten in terms of the local density $\rho(r)$. Taking the polarization operator (6) at the on-shell pion energy $\omega = m_\pi$,

$$\Pi(\omega) = \Pi_{\text{phen}}(\omega = m_\pi; \rho_p, \rho_n),$$

(8)

together with the absorption part, we recover the traditional form of the (energy independent) s-wave optical potential [4,8],The proton and neutron density distributions $\rho_p(r)$ and $\rho_n(r)$ are given as two-parameter Fermi functions $\rho_j(r) = \rho_{0j}[1 + \exp((r - R_j)/a_j)]^{-1}$. The central density $\rho_{0j}$ is normalized to the total number of protons and neutrons in the nucleus. The proton radii, $R_p$, are extracted from the nuclear charge radii following the analyses of muonic atoms [20], taking into account the finite proton size $\langle r_p^2 \rangle = 0.73 \text{ fm}^2$: $R_p^{205}\text{Pb} = 6.66 \text{ fm}$ and $R_p^{207}\text{Pb} = 6.67 \text{ fm}$. Since the charge radii have not been measured for the complete chain of Pb isotopes, we have interpolated linearly between two neighboring measured isotopes. The diffusion coefficient is taken the same for $^{205,207}\text{Pb}$, $a_p = 0.48 \text{ fm}$. For the neutron radii, we use values from the proton-neutron rms-radius difference as obtained in the Brueckner-Hartree-Fock calculations of Ref. [21]: $R_n^{205}\text{Pb} = 6.94 \text{ fm}$ and $R_n^{207}\text{Pb} = 6.97 \text{ fm}$. We assume $a_n = a_p$. The numerical input is close to that in Refs. [3,7].

Solutions of the wave equation (4) for Pb isotopes with the energy independent (threshold) input (8) for the pion-nucleon optical potential are shown in Fig. 1 by open circles. The filled circles in Fig. 1 are the results obtained with the polarization operator,

$$\Pi(\omega) = \Pi_{\text{phen}}(\omega; \rho_p(r), \rho_n(r)),$$

(9)

in which we keep the explicit energy dependence as given by the driving terms (1). The energy dependence effects are evidently important, moving the calculated results closer to the data. Indeed, with the gauge invariant introduction of the electromagnetic interaction in the pion

FIG. 1. Binding energies and widths of deeply bound pionic states in the isotopes $^{207}\text{Pb}$ (left figure) and $^{209}\text{Pb}$ (right figure). Diamonds show the experimental data from [1]. Uncertainties in the extraction of the $1s$ level for $^{207}\text{Pb}$ are indicated by different choices of a control parameter $R$ as specified in [1]. The results for the polarization operator (8) and (9) are depicted by open and filled circles, respectively. Triangles show the results obtained with the chiral polarization operator (10).
polarization operator [via the replacement \( \omega \rightarrow \omega - V_\nu (r) \)], the off-shell pion-nucleon scattering amplitudes are probed at energies \( \omega - V_\nu (r) > m_\pi \). This increases the repulsion in \( T^+ (\omega) \) and disbalances the cancellation between the sigma term \( \sigma_N \) and the range term \( - \beta \omega^2 \) in \( T^+ (\omega) \), giving \( T^+ (\omega - V_\nu (r)) < 0 \). Omitting the replacement \( \omega \rightarrow \omega - V_\nu (r) \) in \( \Pi (\omega) \), we would have \( \omega < m_\pi \), and this would reduce the repulsion in \( T^+ (\omega) \) and turn on attraction in \( T^+ (\omega) \), thus leading in the wrong direction. Taking both the energy dependence and the proper gauge invariant substitution via \( \Pi (\omega - V_\nu (r)) \) is therefore an essential ingredient.

After these qualitative considerations, we proceed now to the systematic calculation of the pion polarization operator using in-medium chiral perturbation theory. Here we extend the results of Ref. [16] at the two-loop level by taking into account the explicit (off-shell) energy dependence. The polarization operator has the form

\[
\Pi (\omega) = \Pi_0 (\omega) + \Pi_{db} (\omega) + \Pi_{rel} (\omega) + \Pi_{cor} (\omega). \tag{10}
\]

The first term corresponds to the linear density approximation:

\[
\Pi_0 (\omega) = -T^- (\omega) \delta \rho - T^+ (\omega) \rho. \tag{11}
\]

The isospin-even off-shell \( \pi N \)-scattering amplitude at zero pion momentum can be written in the following form (for \( \omega > m_\pi \)):

\[
T^+ (\omega) = \frac{\sigma_N - \beta \omega^2}{f^2_\pi} + \frac{3g_\pi^2 m_\pi^2}{16\pi f^4_\pi} + \frac{3g_\pi^2 Q^2 m_\pi^2}{64\pi f^4_\pi} + iT^\text{im},
\]

where \( \beta = g_\pi^2/4M - 2c_2 - 2c_3, \sigma_N = -4c_1 m_\pi^2 - 9g_\pi^2 m_\pi^2/64\pi f^2_\pi \), and \( T^\text{im} = \omega^2 Q/(8\pi f^4_\pi) \). The nucleon axial-vector coupling constant has the value \( g_A = 1.27 \). We introduce the abbreviation \( Q = \sqrt{\omega^2 - m_\pi^2} \). The second-order low-energy constants \( c_{1,2,3} \) (for notations, see Ref. [22]) are tuned to the empirical values of the sigma term [18], \( \sigma_N = 45 \text{ MeV} \), and the \( \pi N \) scattering length, \( T^+ (m_\pi) = 0 \).

The parameter \( \zeta \) reflects freedom in the choice of the interpolating pion field in the effective chiral Lagrangian [13,23]. It enters all interaction vertices with three and more pions. The one-loop correction to the (off-shell) pion self-energy in vacuum depends also on this parameter \( \zeta \). By requiring that the residue at the pion pole remains equal to one [24] as it is implicit in the form of the KG equation (4), one gets the constraint \( \zeta = 0 \).

The isospin-odd off-shell \( \pi N \)-amplitude at zero-momentum reads

\[
T^- (\omega) = \frac{\omega^2}{2f^2_\pi} [1 + \frac{\gamma \omega^2}{(2\pi f^2_\pi)^2} - \frac{\omega^2 Q}{8\pi f^4_\pi} \ln \frac{\omega + Q}{m_\pi} + \frac{i}{2} T^\text{im}], \tag{12}
\]

with \( \gamma = (g_\pi^2 f_\pi/M)^2 + \ln(2\Lambda/m_\pi) \). The cutoff scale \( \Lambda = 737 \text{ MeV} \approx 8f_\pi \) is chosen to reproduce the central empirical value of the on-shell scattering amplitude at threshold \( T^- (m_\pi) = 1.85 \pm 0.09 \text{ fm} \) [19]. We neglect here small additional counterterm contributions proportional to the third order low-energy constants \( \tilde{d}_j \) of Ref. [25].

The next term in (10) corresponds to the important Ericson-Ericson double-scattering correction [2] generalized to isospin asymmetric nuclear matter and off-shell pions:

\[
\Pi_{db} (\omega) = -\square \frac{\omega^2}{3(4\pi f^4_\pi)^4} \left\{ L(k_p, k_p, Q) + L(k_n, k_n, Q) + 2L(k_p, k_n, Q) \right\}, \tag{13}
\]

where \( k_{p,n} = (3\pi^2 \rho_{p,n})^{1/3} \) refer to the proton and neutron Fermi momenta and

\[
L(k_p, k_n, Q) = 4k_p k_n (Q^2 + 3k_p^2 + 3k_n^2) + 8Q(k_p^2 - k_n^2) + 3(k_p^2 - k_n^2)^2 + 6Q^2 (k_p^2 + k_n^2) - Q^4 \left| \ln \frac{(Q^2 - k_p^2)^2 - Q^2}{(k_p + k_n)^2 - Q^2} \right|.
\]

The third term in (10) is a small relativistic correction from the particle-hole (Born) diagram evaluated at zero pion momentum:

\[
\Pi_{rel} (\omega) = \square \frac{g_A^2 \omega}{10\pi M f^2_\pi} (k_p^5 - k_n^5). \tag{15}
\]

The last term in (11) represents the effect induced by \( \pi \pi \) interactions with two virtual pions being absorbed on the nucleons in the Fermi sea, and by an additional two-loop correction [16,23]:

\[
\Pi_{cor} (\omega) = \square \frac{g_A^2}{20(4\pi f_\pi)^4} \times \left\{ (Q^2 (\zeta + 2) + 5m_\pi^2)[H(k_p, k_p) + H(k_n, k_n)] + Q^2 (8\zeta - 4) H(k_p, k_n) \right\}. \tag{16}
\]

The function \( H(k_p, k_n) \) consists of the last four terms
written in Eq. (12) of Ref. [16]. In the actual calculation, the contribution \( \Pi_{\text{corr}}(\omega) \) turns out to be negligibly small.

Solutions of the wave Eq. (4) for \( 1s \) and \( 2p \) levels using (10) are shown in Fig. 1 by triangles. They agree well with experimental data. We also find that the energy dependent polarization operator (6) and (7) gives equally good results as (10) if the amplitude \( T(\omega) \) in (1) is extended to include the \( \omega^4 \) term in (12), with the parameter \( \gamma \) tuned to the empirical value of the scattering length.

In Fig. 2, we examine the dependence of our results for \( ^{205}\text{Pb} \) on the less constrained parameters of the model. Variations of the neutron radius \( R_n \) affect mainly the binding energy, whereas the sigma term \( \sigma_N \), \( \text{Im} B_0 \), and \( \text{Re} B_0 \) have a stronger impact on the level width. Note the strong correlation in the effects induced by changes of \( \text{Re} B_0 \) and \( \sigma_N \). Finally, we mention that the new data on three Sn isotopes [26] can provide an additional check for our approach. The corresponding analysis will be presented elsewhere.

In summary, we have demonstrated that the long-standing issue of the missing repulsion in the \( s \)-wave pion-nucleus potential can be at least partially resolved by taking into account the explicit energy dependence of the pion self-energy and the gauge invariant incorporation of electromagnetic interactions. The experimental data for \( 1s \) and \( 2p \) levels in Pb isotopes are well reproduced. We also have clarified that, to leading order, the energy dependence effects in the pion polarization operator can be interpreted in terms of an in-medium reduction of the pion decay constant, entering in an equivalent, energy independent optical potential.

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[23] We discard here the fact the wave function renormalization factor of the pion in vacuum receives also the contribution \(-2l_4m_n^2f_\pi^2\) from the low-energy constant \(l_4\).