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 $^{205}$Pb and $^{207}$Pb are well reproduced, and the notorious ”missing repulsion” in the pion-nuclear s-wave optical potential is accounted for. 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 [7] have set new standards and constraints for the detailed analysis of s-wave pion-nucleus interactions. This subject has a long history [2, 3, 4, 5, 6, 7, 8], culminating in various attempts to understand the ”missing repulsion” [9]. The spontaneous and explicit breaking of chiral symmetry implies the following leading terms of those amplitudes [13]:

\[
T^+(\omega) = \frac{\sigma_N - \beta \omega^2}{f^2_{\pi}}, \quad T^-(\omega) = \frac{\omega}{2f^2_{\pi}},
\]

where $f_{\pi} = 92.4$ MeV is the pion decay constant, $m_\pi = 139.57$ MeV is the (charged) pion mass and $\sigma_N \approx 45 \pm 8$ MeV is the pion-nucleon sigma-term. The empirical observation that $T^+(m_\pi) = (0.04 \pm 0.09) \text{ fm} \approx 0$ sets the constraint $\beta \simeq \sigma_N/m^2_\pi$.

Next, consider the pionic in-medium dispersion equation at zero momentum, $\omega^2 - m^2_\pi - \Pi(\omega) = 0$. Introduce an (energy independent) equivalent optical potential $U$ by $\omega^2 = m^2_\pi + 2m_\pi U$ with $U \ll m_\pi$, and expand around $\omega = m_\pi$. This gives

\[
U \simeq \frac{\Pi(m_\pi)}{2m_\pi} \left(1 + \frac{\Pi'(m_\pi)}{2m_\pi}\right) + \ldots \simeq \frac{\Pi(m_\pi)/(2m_\pi)}{1 - \frac{\Pi(m_\pi)}{2m_\pi}}\bigg|_{\omega=m_\pi},
\]

where the last approximate step introduces the wave function renormalization factor $1 - \frac{\Pi(m_\pi)}{2m_\pi}$. The difference between second and last step in [13] is of sub-leading order. Inserting [11] and assuming $\delta \rho \ll \rho$ one finds

\[
U \simeq -\frac{\delta \rho}{4f^2_{\pi}} \left(1 - \frac{\sigma_N \rho}{m^2_\pi f^2_{\pi}}\right)^{-1} \simeq -\frac{\delta \rho}{4f^2_{\pi}},
\]

which is the expression proposed in ref. [12]. It involves the driving Weinberg-Tomozawa term in $T^-(\omega)$, but with the pion decay constant renormalized $(f_{\pi} \rightarrow f^*_\pi(\rho))$ to leading order in the density $\rho$, 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 $\langle \bar{q} q \rangle$. Of course, rather than constructing the potential $U$ and following the steps leading to the KG equation, 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

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

$$\Delta \Pi_S(\omega; \rho_p, \rho_n) = -8\pi \left(1 + \frac{m_\pi}{2M}\right) B_0 \rho_p \rho_n + \rho_p,$$  (5)

parameterized as in ref. [3]. Here $M$ stands for the nucleon mass. We use $\text{Im} B_0 = 0.063 \text{fm}^{-4}$ and $\text{Re} B_0 = 0$ as our standard set and discuss variations of $\text{Re} B_0$ 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. [3] (set A).

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 [3]. When those are included the "phenomenological" s-wave pion polarization operator becomes [3]:

$$\Pi_{\text{phen}}(\omega; \rho_p, \rho_n) = -T^- (\omega) \delta \rho - T^+ (\omega, \rho, \rho),$$  (6)

with

$$T^+ (\omega, \rho) = T^+(\omega) - \frac{3k_F}{8\pi^2} \left( [T^+(\omega)]^2 + 2 |T^- (\omega)|^2 \right).$$  (7)

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

$$\Pi(\omega) = \Pi_{\text{phen}}(\omega = m_\pi; \rho_p, \rho_n),$$  (8)

we recover the traditional form of the (energy independent) s-wave optical potential [3].

The proton and neutron density distributions $\rho_p(r)$ and $\rho_n(r)$ are given as two-parameter Fermi functions $\rho_j(r) = \rho_{0,j}[1 + \exp((r - R_j)/a_j)]^{-1}$. The central density $\rho_{0,j}$ 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 from the analyses of muonic atoms [19], taking into account the finite proton size $<r_p^2> = 0.73 \text{ fm}^2$: $R_p[{}^{205}\text{Pb}] = 6.66 \text{ fm}$ 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 diffuseness coefficient is taken the same for $^{205,207}\text{Pb}$, $a_p = 0.48 \text{ fm}$. For the proton radii we use values from the proton-neutron rms-radius difference as obtained in the Brueckner-Hartree-Fock calculations of ref. [20]: $R_n[{}^{205}\text{Pb}] = 6.94 \text{ fm}$ 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 [3] for Pb isotopes with the energy independent (threshold) input [3] for the pion-nuclear 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 [3]. 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 polarization operator (via the replacement $\omega \to \omega - V_c(r)$) the off-shell pion-nucleon scattering amplitudes are probed at energies $\omega - V_c(r) > m_\pi$. This increases the repulsion in $T^-(\omega)$ and disbalances the cancelation between the sigma-term $\sigma_N$ and the range term $-\beta \omega^2$ in $T^+(\omega)$, giving $T^+(\omega - V_c(r)) < 0$. Omitting the replacement $\omega \to \omega - V_c(r)$ 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 $\Pi(\omega - V_c(r))$ 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. [3] at the two-loop level by taking into account the explicit (off-shell) energy dependence. The polarization operator has the form:

$$\Pi(\omega) = \Pi_0(\omega) + \Pi_{\text{ds}}(\omega) + \Pi_{\text{rel}}(\omega) + \Pi_{\text{cor}}(\omega).$$  (10)

The first term corresponds to the linear density approximation:

$$\Pi_0(\omega) = -T^- (\omega) \delta \rho - T^+ (\omega) \rho. $$  (11)
The isospin-even off-shell $\pi N$-scattering amplitude at zero pion momentum can be written in the following form (for $\omega > m_\pi$):

$$ T^+(\omega) = \frac{\sigma_N - \beta \omega^2}{f_\pi^2} + \frac{3g_\pi^2m_\pi^2}{16\pi f_\pi^2} + \frac{3g_\pi^2Q^2m_\pi\zeta}{64\pi f_\pi^4} + iT_{\text{im}} $$

where $\beta = g_\pi^2/4M - 2c_2 - 2c_3$, $\sigma_N = -4c_1m_\pi^2 - 9g_\pi^2m_\pi^2/64\pi f_\pi^2$ and $T_{\text{im}} = \omega^2Q/(8\pi f_\pi^4)$. 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. [24]) are tuned to the empirical values of the sigma-term [17], $\sigma_N = 45$ 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, 22]. 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:

$$ T^-(\omega) = \frac{\omega}{2f_\pi^2} \left[ 1 + \frac{\gamma \omega^2}{(2\pi f_\pi)^2} \right] - \frac{\omega^2Q}{8\pi f_\pi^4} \ln \frac{\omega + Q}{m_\pi} + i\frac{1}{2} T_{\text{im}} $$

(12)

with $\gamma = (g_A\pi f_\pi/M)^2 + \ln(2\Lambda/m_\pi)$.

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:

$$ \Pi_{\text{ds}}(\omega) = -\frac{\omega^2}{3(4\pi f_\pi)^4} \left\{ L(k_p, k_p, Q) + L(k_n, k_n, Q) + 2L(k_p, k_n, Q) \right\} . $$

(13)

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

$$ L(k_p, k_n, Q) = 4k_pk_n(Q^2 + 3k_p^2 + 3k_n^2) $$

$$ + 8Q(k_p^2 - k_n^2) \ln \frac{Q + k_n - k_p}{Q - k_n + k_p} $$

$$ - 8Q(k_n^2 + k_p^2) \ln \frac{Q + k_p + k_n}{Q - k_p - k_n} $$

$$ + 3(k_p^2 - k_n^2)^2 + 6Q^2(k_p^2 + k_n^2) - Q^4 \right\} $$

$$ \times \ln \frac{(k_n - k_p)^2 - Q^2}{(k_p + k_n)^2 - Q^2} . $$

(14)

The third term in (11) is a small relativistic correction from the particle-hole (Born) diagram evaluated at zero pion momentum:

$$ \Pi_{\text{rel}}(\omega) = -\frac{g_\pi^2\omega}{10(\pi M f_\pi)^2} (k_p^5 - k_n^5) . $$

(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 [14, 22]:

$$ \Pi_{\text{cor}}(\omega) = -\frac{g_\pi^2}{20(4\pi f_\pi)^4} $$
medium reduction of the pion decay constant, or equivalently, the renormalization of the intrinsic pion wave function in matter.

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FIG. 2: Dependence of energies and widths of pionic levels for $^{205}$Pb on parameters of the optical potential. Solid lines correspond to the variation of the neutron radius in the interval $\delta R_n = -0.2 \pm 0.2$ fm. Dashed lines show the variation with the pion nucleon sigma term $\sigma_N(0) = 20 \pm 65$ MeV. Dotted lines represent the variation of $\text{Re} B_0 = (-0.5 \pm 0.5) \text{Im} B_0$. Arrows indicate the directions in which results move as the varied parameters increase. Triangles and experimental points are the same as in Fig. 1.

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 $\Pi_{\text{cov}}(\omega)$ turns out to be negligibly small. Solutions of the wave equation (4) for 1s and 2p levels using (16) are shown in Fig. 1 by triangles. They agree well with experimental data. We also find that the energy dependent polarization operator (15) gives equally good results as (14) if the amplitude $T^{-}(\omega)$ in (14) is extended to include the $\omega^3$ 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 $^{205}$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 $\sigma_N$ 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 $\sigma_N$.

In summary, we have demonstrated that the long standing issue of the "missing repulsion" in the s-wave pion nucleus potential can be naturally 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 have also clarified that, to leading order, the energy dependence effects can be interpreted in terms of the intrinsic 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.

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\[ \times \left\{ (Q^2(\zeta + 2) + 5m^2_\pi)H(k_p, k_n) + H(k_n, k_n) \right\} . \]