Extracting free-space observables from trapped interacting clusters

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The energy spectrum of two short-range interacting particles in a harmonic potential trap has previously been related to free-space scattering phase shifts. But the existing formula for this purpose is exact only in the limit of an infinitely shallow trap. Here we provide a systematically improved formula—describing the low-energy dynamics—that enables the use of finite traps. This paves the way for extracting nuclear scattering phase shifts from ab initio nuclear many-body structure calculations, a long-sought goal in nuclear physics. The derivation establishes effective field theory as a powerful framework for studying the connection between structure information of a trapped system (with two or more sub-clusters) and continuum physics in the fields of both nuclear and condensed-matter physics.

Introduction

Nuclear experiments at low energy can not manipulate many-body systems to the extent possible in condensed-matter or cold-atom experiments. However, with progress in many-body methods [1–5] and increasing computing power (and quantum computers [6]), we can start manipulating nuclear systems computationally. Here we show how trapping two clusters at low energy in a harmonic potential well tells us about their free-space scattering through a formula connecting low-energy phase shifts with the confined spectrum. In this approach the trap compacts the system and reduces the required degrees of freedom enough to allow controlled ab initio calculations, as will be demonstrated elsewhere. (See e.g., [7–10] for other ab initio approaches of computing light-nucleus scatterings.)

A formula for particles in the infinitely-shallow trap was derived in Ref. [11], and later generalized to include the full energy dependence of the phase-shift (besides the scattering length term in [11]) and for partial waves beyond s-wave [12–20]. The result for angular momentum ℓ [17, 18, 21] (called the BERW formula here) is

\[ p^{2\ell+1} \cot \delta_{\ell}(E) = (-)^{\ell+1}(4M_n\omega)^{\ell+\frac{1}{2}} \frac{\Gamma\left(\frac{3}{4} + \frac{\ell}{2} - \frac{E}{\omega}\right)}{\Gamma\left(\frac{1}{4} - \frac{\ell}{2} - \frac{E}{\omega}\right)}. \]

This holds at the eigenenergies \( E \equiv p^2/2M_n \)—with the center-of-mass (CM) energy subtracted—in a trap where each particle experiences a potential \( \omega^2 r^2/2 \) times its mass; \( M_n \) is the reduced mass and \( \delta_{\ell} \) the phase shift. Equation (1) is analogous to the Luscher formula [22, 23] that is widely applied in Lattice Quantum Chromodynamics (for a system on a space-time torus).

Refs. [21, 24] have used Eq. (1) to extract nuclear scattering from ab initio spectrum calculations. However, away from the infinitely-shallow-trap limit (i.e., for \( \omega \neq 0 \)), Eq. (1) does not capture the external potential’s modifications to the interaction at short distances. To illustrate the impact on extracting phase shifts, we use a two-body potential model [25] designed for describing neutron-α scattering [see the supplemental materials (SM) for details]. Figure 1(a) shows 3/2− p-wave phase shifts extracted using Eq. (1) at the \( \omega \)-dependent eigenenergies. The “True” curves are the exact phase shifts. (b) After subtracting \( \omega \)-dependent pieces from generalized ERE curves (inset), the extractions from Eq. (2) lie on the “True” curve.

Here we remedy the BERW formula using pionless effective field theory (EFT) [26–28], which enables low-energy dynamics to be studied without specifying the details of the short-distance physics (e.g., potential or cluster structure and excitation). This EFT was used to re-derive and generalize the Luscher formula [23, 29]. The improved formula for a harmonic trap is

\[ \sum_{i,j=0}^{\infty} C_{i,j} (M_n \omega)^{2i} p^{2j} = (-)^{\ell+1}(4M_n\omega)^{\ell+\frac{1}{2}} \frac{\Gamma\left(\frac{3}{4} + \frac{\ell}{2} - \frac{E}{\omega}\right)}{\Gamma\left(\frac{1}{4} - \frac{\ell}{2} - \frac{E}{\omega}\right)} \]

\[ \times \sum_{j=0}^{\infty} C_{i=0,j} p^{2j}. \]

The constants \( C_{i,j} \) depend implicitly on \( \ell \) but are independent of \( \omega \) and \( p \); they are dimensionful and scale as...
proper powers of a high-momentum scale $M_H$ (as dictated by, e.g., the cluster excitations), unless there is fine tuning. The series sum can be truncated with a controlled error when $\sqrt{M_n \omega}$ and $p$ are smaller than $M_H$.

To infer the phase shifts from Eq. (2) given the eigenenergies, the $C_{i \neq 0,j}$ terms, which capture the trap-induced modifications, must be simultaneously calibrated with the $C_{0,j}$. The latter determine the free-space phase shifts via the effective range expansion (ERE) [26, 28]. Knowing the full potential in the n-α model, we can fix $C_{i,j}$ (see the SM) and generate Fig. 1(b): the inset shows that the phase shifts extracted from Eq. (1) for a given $\omega$ sit on a curve parameterized by a generalized ERE, in which the $j$th-order coefficient is given by $\sum_{i=0}^{j} C_{i,j}(M_n \omega)^{2i}$. After subtracting the trap-induced modifications, the extracted phase shifts agree with the “True” curve.

To extract nuclear phase shifts (or $C_{i,s}$) from $ab$ initio spectra, Eq. (2) will play a crucial role, because $ab$ initio calculations, developed to computing compact nuclear spectra, Eq. (2) will play a crucial role, because $ab$ initio calculations, developed to computing compact nuclear spectra. To infer the phase shifts from Eq. (2) given the eigenenergies, the $C_{i \neq 0,j}$ terms, which capture the trap-induced modifications, must be simultaneously calibrated with the $C_{0,j}$. The latter determine the free-space phase shifts via the effective range expansion (ERE) [26, 28].

The building blocks of $\mathcal{L}_0$, $\mathcal{L}_1$ are invariant under rotation and Galilean translation [32]: (1) for $\psi = n, c$, or $\phi, \psi^\dagger \hat{i} \psi + \hat{\phi}^\dagger / \sqrt{2} V \psi / \sqrt{2}$; (2) the $g_{\ell}$ coupling in $\mathcal{L}_1$ uses $n$-$c$'s relative velocity $\mathbf{V}$, while $V^{\otimes \ell}$ denotes a rank-$\ell$ operator composed of $\ell$ copies of $V$ normalized such that when $m_\ell = \pm \ell, [V^{\otimes \ell}]_{m_\ell} = [(V^{\otimes \ell})^*]_{\ell} = -V^{\otimes \ell}$. (i.e., $\phi^{m_\ell}$ is coupled to a $n$-$c$ configuration having $\ell$ and $m_\ell$ as its relative angular quantum numbers). The short-distance interactions in $\mathcal{L}_0$ and $\mathcal{L}_1$ follow closely previous works using a dimer-field approach [27–29, 31, 33, 34]: $\sigma_\ell (= \pm 1, \Delta_\ell, g_{\ell}$, and $d_{\ell}^{(l)}$ together reproduce the ERE (see Eq. (6) and [29, 34]). Repeated indices in the Lagrangian (and in Eqs. (6), (8), and (9)) are implicitly summed with specified ranges.

Other vertices coupling $\mathcal{B}$ and the particles are severely constrained, thanks to a unique property of a harmonic potential: the CM of a multi-particle system is decoupled from its internal dynamics [35]. For $d_{j,k}^{(l)}$ couplings with $M_n^2 \mathbf{B}^2 \mathcal{B} / (3m) = M_n^2 \omega^2, \mathbf{B}$ ensures that they only shift the system’s energy by $r$-independent but $\omega^2$-dependent functions so that the CM behaves as a free particle in traps. Structures such as (1) $\mathcal{B}^2, \mathcal{B}^3, \ldots (2) (\partial \mathcal{B})^4, (\partial \mathcal{B})^6, \ldots [(\partial \mathcal{B})^2$ can be absorbed into the $\phi^\dagger$ coupling in $\mathcal{L}_0$ and (3) products of (1) and (2) would all distort the CM’s motion. Derivatives higher than $\mathbf{B}^2$ applied on $\mathcal{B}$ would give zero. In the free space, defining energy relative to the $n$-$c$ threshold sets $\Delta_\ell = \Delta_n = 0$. Both are modified by $\mathcal{B}$ through “polarization” effects as $\Delta_\ell$ by $d_{j=0,k}^{(l)}$ couplings, but they only affect the energy-references in traps and for simplicity not shown here.

In principle $\mathcal{B}$ can be coupled to the $\phi^{m_\ell}$ operators (e.g., the $g_{\ell}$ term), which again must take the form of $(\partial \mathcal{B})^{1/2} \ldots$. However, these terms can be eliminated by rescaling the $\phi$ field by $1 + \mathbf{B}^2 (M_n \omega)^2 \ldots$. Since the rescaling-induced terms are already present as $d_{j,k}^{(l)}$ couplings in $\mathcal{L}_1$, the trap modification to $g_{\ell}$ is not included.

To compute the propagator of the dimer $\phi$, its self-energy correction due to $n$-$c$ multiple scattering needs to be included. A cut-off on momentum is applied to regularize loops in free space, while in traps the cut-off is applied on the virtual excitation energy [26]. (However, for fine-tuned systems other schemes would be preferred, e.g., power divergence
subtraction [36].) Within time-independent perturbation theory [30], the one-loop self-energy bubble diagram in free space is \((2\pi)^3\delta(P - P')\delta_{m' j}^m \Sigma(E_L, P)\equiv \langle \phi_{P'}^m | H_{qf} (E_L - H_0 + i\nu^{-1})^{-1} H_{gf} | \phi_{P}^m \rangle\). \(H_0\) and \(H_{gf}\) are the Hamiltonians derived from \(\mathcal{L}_0\) and the \(q_f\) term in \(\mathcal{L}_1\), respectively [30]. Both states are plane waves, with \(P, P', E_L, m_e,\) and \(m'_i\) as \(\phi\)'s momenta and energy in the Lab frame, and its spin projections. We then obtain

\[
\Sigma(E) = \frac{\delta\ell}{\pi} \int_0^{T_\Lambda} \frac{d T_q}{E - T_q} \frac{(2M_\text{H} T_q)^{\ell' + \frac{1}{2}}}{E - T_q + i\nu^+} \equiv -\delta\ell \left\{ p^{2\ell + 1} + \sum_{j=0}^{+\infty} L_{\ell,j}(\Lambda) p^{2j} \right\},
\]

\[
\Sigma(E) = \frac{g^2_\text{f}}{M_\text{H}^{2\ell - 1}} \frac{2\ell' - 2\ell + 1}{\pi(2\ell + 1)!} L_{\ell,j}(\Lambda) = \frac{2\Lambda^{2\ell - 2\ell + 1}}{\pi(2\ell - 2\ell + 1)}. \tag{5}
\]

\(p \equiv \sqrt{2M_\text{H} (E + i\nu^{-1})}, \ T_q \equiv q^2/(2M_\text{H}), \ \Lambda\) is the cut-off on \(|q|, \ T_\Lambda \equiv \Lambda^2/(2M_\text{H}), \ E \equiv E_L - P^2/(2M_\text{H})\) as the energy in the CM frame. Note \(L_{\ell,j}(\Lambda) \rightarrow 0\) as \(\Lambda \rightarrow \infty\).

The fully dressed free-space \(\phi\) propagator, which is defined through \((2\pi)^3\delta(P - P')\delta_{m' j}^m D(E_L, P)\equiv \langle \phi_{P'}^m | H_{L} (E_L - (H_0 + H_1) + i\nu^+)^{-1} H_{P} | \phi_{P}^m \rangle\), with \(H_1\) from \(\mathcal{L}_1\), can be computed by summing the self-energy-insertion diagrams due to \(\Sigma\) and the \(d_{j,\ell}^{(j)}\) vertices, yielding

\[
D = \frac{1}{\sigma\ell(E + \Delta\ell) - d_{j,\ell}^{(j)} E_j - \Sigma} = -\frac{\delta\ell^{-1}}{p^{2\ell + 1} [\cot \delta\ell - i]},
\]

with \(p^{2\ell + 1} \cot \delta\ell = \sum_{j=0}^{+\infty} C_{0,j} p^{2j}\), and

\[
C_{0,j} = \frac{\delta\ell^{-1}}{(2M_\text{H} \Lambda)^j} \left\{ -\sigma\ell \Delta\ell, -\sigma\ell, d_2^{(j)}, d_4^{(j)}, \ldots \right\} L_{\ell,j}(\Lambda). \tag{6}
\]

\(D\) is related to \(\delta\ell\) through the scattering \(T\)-matrix, which is computed by multiplying \(D\) with two \(g_e\)-vertices [30]. The range of the index in \(d_{j,\ell}^{(j)}\) in the implicit sum is fixed in \(\mathcal{L}_1\), and in the \(C_{0,j}\) definition \(\ldots\) \(j\) is the \(j\)th component of the list and \(j\) is not summed.

Now let us turn to the trapped system. Based on \(\mathcal{L}_0\), we can expand \(n, c\) and \(\phi\) fields using their corresponding harmonic-oscillator wave functions [18]. Again note that the \(g_q\) coupling only picks up the \(n\)-\(c\) configuration whose total angular momentum and projection equal those of the CM motion (i.e., \(\phi\)) and whose relative angular momentum and projection equal the \(\phi\)'s spin and projection \((\ell\) and \(m_\ell\)). Thus the matrix element between \(\phi\)'s eigenstates in a trap for defining its self-energy becomes \(\delta_{n_c} n'_{m'} \Sigma_\omega(\ell) \equiv \langle \phi_{n_c} \phi_{n_c} | H_{qf} (E_L - H_0)^{-1} H_{gf} | \phi_{n'_{m'} c} \rangle\) (note the absence of \(i0^+\) in the Green's function), with

\[
\Sigma_\omega(\ell) = \frac{g^2_\text{f} (2\ell + 1)!}{M_\text{H}^{2\ell + 2\pi}} \sum_{n=0}^{n\Lambda} \left( \frac{\tilde{R}_{n,\ell}(0)}{E - E_{n,\ell}^{(r)}} \right)^2 = \frac{\delta\ell}{\pi} \left( 4M_\text{H} \omega \right)^{\ell' + \frac{1}{2}} \sum_{n=0}^{n\Lambda} f_\ell (z_\ell, n), \tag{7}
\]

\[
f_\ell (z_\ell, n) = \frac{\Gamma(n + \ell + \frac{3}{2}) \Gamma(n + 1)}{z_\ell^n (n + \ell + \frac{3}{2})}. \tag{7}
\]

Here \(z_\ell \equiv E/(2\omega)\) and the relative energy \(E \equiv E_L - E_{\phi}^{(\ell)}\) with \(E_{\phi}^{(\ell)} = (2N_\phi + \ell + \frac{3}{2})\omega\) as the CM's energy. If \(\Delta_\phi\) and \(\Delta_n\) receive trap-dependent “polarization” corrections, these corrections also need to be subtracted in defining \(E\). In the derivation, a unitary transformation between \(n\) and \(c\) single-particle and CM:relative motion eigenmodes has been used.

Summing over the quantum numbers associated with the intermediate state’s CM motion gives rise to the \(\delta_{n_c} n'_{m'}\) factor in defining \(\Sigma_\omega\), since the CM’s decoupling property is preserved and thus so is \(N_\phi\). For the relative dynamics, \(R_\ell^{(r)}(\tau)\) is part of the eigenmode function \(R_\ell^{(r)}(\tau)\) [18]: \(R_\ell^{(r)}(\tau) \equiv \bar{R}_\ell^{(r)}(\tau) \gamma Y_{m_\ell}(\tau)\). \(N_c\) has \(n, \ell\) for its radial excitation and angular momentum, and \(E_{n,\ell}^{(r)} = (2n + \ell + \frac{3}{2})\omega\). A cut-off on \(n\) is used to regularize the theory in a trap, which is in place with the regularization used in Eq. (5).

The \(\phi\) propagator in the trap, defined as \(D_\omega(E)\delta_{n_c} n'_{m'}\), can be computed by summing up all self-energy insertion diagrams, including insertions of \(\Sigma_\omega\) and those of the \(d_{j,\ell}^{(j)}\) and \(d_{j,k}^{(j)}\) vertices. We get

\[
D_\omega = \frac{1}{\sigma\ell(E + \Delta\ell) - d_{j,\ell}^{(j)} E_j - \Sigma_\omega(E) - d_{j,k}^{(j)} E_j (M_\text{H} \omega)^{2k}}. \tag{8}
\]

In Eq. (8) to zero:

\[
p^{2\ell + 1} \cot \delta\ell + \frac{d_{j,k}^{(j)} E_j (M_\text{H} \omega)^{2k}}{\delta\ell} = \frac{\partial \Sigma(\ell) - \Sigma_\omega(\ell)}{\delta\ell}, \tag{9}
\]

There exists a special relation between \(\Lambda\) and \(n_\Lambda\) such
that the divergences in $\Sigma$ and $\Sigma_\omega$ cancel in Eq. (9), and thus $d_{j,k}^{(l)}$ are finite. This should be considered as a specific scheme. The right side of Eq. (9) becomes

$$\begin{align*}
-\frac{1}{\pi} (4M_n \omega)^{l+\frac{1}{2}} & \left[ \sum_{n=0}^{n_A} f_{\ell} (z_E, n) + \frac{\ell}{2} \sum_{j=0}^{\ell} z^j E (\bar{L}_{1,j} \sqrt{\frac{\bar{T}_A}{2}}) \right] \\
\equiv -\frac{1}{\pi} (4M_n \omega)^{l+\frac{1}{2}} & \sum_{n=0}^{(\mathcal{R})} f_{\ell} (z_E, n).
\end{align*}$$

(10)

Here, $a(\mathcal{R})$ labels the renormalized series sum with $n_A \to +\infty$; $\bar{T}_A \equiv T_{\Lambda}/\omega$. To derive this $n_{\Lambda}-\Lambda$ relation, the $n_{\Lambda}$-dependence of $\Sigma_\omega$ needs to be studied.

Two formulas are useful for understanding $f_{\ell}(z_E, n)$ at large $n$ and $\Sigma_\omega$ at large $n_{\Lambda}$. The first is [37, Eq. 5.11.13]

$$\frac{\Gamma(z+a)}{\Gamma(z+b)} \sim \frac{\infty}{\sum_{k=0}^{\infty} G_k (a, b)} \text{ if } \arg(z) \leq \pi - 0^+.$$  

(11)

Here $a$ and $b$ are real or complex constants, and $G_k (a, b)$ as a function of $a$ and $b$ is related to the generalized Bernoulli polynomials [37, Eq. 5.11.17] [38]. The second is the Euler-Maclaurin formula [37, Eq. 2.10.1], stating that for a smooth $f(x)$, its series sum can be approximated using an asymptotic expansion:

$$\sum_{n=0}^{n_A} f_{\ell}(0, n) = \int f(x) dx + f(n_{\Lambda}) + \frac{1}{2} B_{2j} \frac{d^{2j-1} f(n_{\Lambda})}{dn_{\Lambda}^{2j-1}}.$$  

(12)

where $B_{2j}$ is a Bernoulli number. Only the $n_A$ dependent terms are shown. Like $\Sigma(E)$, the $0^{\text{th}}$ to $6^{\text{th}}$ derivatives of $\Sigma_\omega(E)$ diverge. So for s-waves, only $\Sigma_\omega(0)$ is considered:

$$\sum_{n=0}^{n_A} f_{\ell}(0, n) = \sum_{n=0}^{n_A} \frac{1}{\sqrt{n}} \left[ 1 + O \left( \frac{1}{n} \right) \right] \sim -2n_{\Lambda}^\frac{1}{2} + O(n_{\Lambda}^{-\frac{1}{2}}).$$

(13)

Thus $\bar{T}_A = 2n_{\Lambda} (1 + O(n_{\Lambda}^{-\frac{1}{2}}))$ so that the divergence can be absorbed by $\sqrt{2\Lambda A}$ in Eq. (10). The $O(n_{\Lambda}^{-\frac{1}{2}})$ term in the $n_{\Lambda}-\Lambda$ relation is not relevant when $n_{\Lambda} \to \infty$. For p-waves, the $0^{\text{th}}$ and first derivatives are divergent:

$$\begin{align*}
\sum_{n=0}^{n_A} f_{\ell=1} (0, n) & \sim -\frac{2}{3} n_{\Lambda}^{-\frac{3}{2}} - \frac{7}{4} n_{\Lambda}^{-\frac{1}{2}} + O \left( n_{\Lambda}^{-\frac{3}{2}} \right), \\
\sum_{n=0}^{n_A} \partial_{z_E} f_{\ell=1} (z_E, n) |_{z_E=0} & \sim -2n_{\Lambda}^{-\frac{1}{2}} + O \left( n_{\Lambda}^{-\frac{3}{2}} \right).
\end{align*}$$

(14)

(15)

Thus, $\bar{T}_A = 2n_{\Lambda} (1 + \frac{7}{4} n_{\Lambda}^{-\frac{3}{2}} + O(n_{\Lambda}^{-\frac{5}{2}}))$, to have these divergences canceled by those in $\mathcal{P} \Sigma(E)$ in Eq. (10).

The $n_{\Lambda}^{-\frac{1}{2}}$ piece in the expression must be specified, but higher-order terms are not needed. However for d-waves, another order higher needs to be specified: $\bar{T}_A = 2n_{\Lambda} (1 + \frac{7}{4} n_{\Lambda}^{-\frac{3}{2}} + \frac{\gamma}{32} n_{\Lambda}^{-1} + O(n_{\Lambda}^{-3}))$; for even larger $\ell$, more terms need to be specified accordingly.

This requirement is tied to the fact that for a specific $E$-derivative, there is a tower of divergences with different degrees in $\Sigma_\omega$ (e.g., Eq. (14)), in stark contrast with the same derivative of $\Sigma$, where the power of $\Lambda$ is fixed by the the dimensions. Any alternative $n_{\Lambda}-\Lambda$ relation would need to ensure that the divergences in Eq. (9)’s right side can be absorbed by the $d_{j,k}^{(l)}$ terms in the left side so that phase shifts are cut-off independent and the CM-decoupling property is not violated.

To finish this derivation, this identity is needed:

$$\sum_{n=0}^{(\mathcal{R})} f_{\ell}(z_E, n) = (-)^{\ell} \pi \left( \frac{4 + 3}{\pi} \right)^{\frac{4 - \ell}{2}},$$

(16)

which holds in the entire complex $z$ plane (both sides have the same poles and residues, see the proof in the SM). By redefining $d_{j,k}^{(l)} \equiv \mathcal{A}_k (2M_R)^{\ell} C_{i,j}$ in Eq. (9) and applying Eq. (16) in Eq. (10), Eq. (9) gives Eq. (2).

Further comments It is worth comparing $D(E)$ in Eq. (6) and $D_{\omega}(E)$ in Eq. (8) in the complex $E$ plane. $1/D(E)$ has a branch cut—known as the unitary cut—on the positive real axis due to the $-i p^{2\ell+1}$ term, which changes into a series of poles—called “unitary” poles below—for $1/D_{\omega}(E)$ (from the term $[\Sigma_\omega(E) - \mathcal{P} \Sigma(E)]/\mathcal{A}_k$). Both non-analyticities are directly connected to unitarity and thus independent of framework, power counting, and fine tuning.

However, fine tuning and power counting do impact the behavior of EREs, as shown in Ref. [26] using EFTs without a dimer field: in a natural case, $C_{0,3} \sim M^{4+1-2j}$; in a 1st fine-tuned case, $C_{0,0}$ is enhanced; and in a 2nd fine-tuned case, the ERE has low-energy poles. Based on this work, we can include the couplings between $\mathcal{B}(x)$ and particles in those EFTs and compute the $T$-Matrix in a trap. Again, the new Lagrangian terms are in the form of the original short-distance-interaction terms multiplied by $(\mathcal{P} \mathcal{B})^{1/2}$, which in effect amounts to modifying the original EFT bare couplings by adding polynomials in $\omega^2$ as corrections.

For all three cases, the resulting $T$-Matrix is the four-space $T$-Matrix in Ref. [26] with the original bare couplings substituted by the corresponding modified ones and the unitary cut by the “unitary” poles. Identifying the poles of the trap $T$-Matrix gives a similar quantization condition as Eq. (9). For the natural and the 1st fine-tuned case, we reproduce Eq. (1). For the 2nd fine-tuned case, a Laurent expansion of $p^{2\ell+1} \cot \delta$ was derived [26], so the same expansion should be used in Eq. (2) with the parameters carrying $\omega^2$ corrections.

In other words, resumming of $d_{j,k}^{(l)}$ and $d_{j,k}^{(l)}$ terms is needed.

Summary We have applied pionless EFT to two short-range interacting particles in an external harmonic trap to derive a systematically improved BERW formula that is exact even at finite $\omega$. It is valid when the infrared scale of the trap $(\sqrt{M_R} \omega)$ and the relative momentum ($p$) are both smaller than the high momentum scale set by the dynamics. This provides a firm foundation for implementing a Luscher-formula-like approach to
connect nuclear scattering and \textit{ab initio} structure calculations. The derivation involved new coupling terms between the background field and particles, which lead to the improvements of the original BERW formula. Moreover, a careful analysis of renormalization shows a non-trivial relation between the cut-off $\Lambda$ on relative momentum in free space and cut-off $n_A$ on the number of radial excitation in a trap. The renormalization procedure is further confirmed by Eq. (16)’s proof. Both aspects are instructive for deducing connections between a trapped system (with two or more clusters) and free-space scattering/reactions for both nuclear and cold atom physics [20]. It should also be interesting to apply this framework to study exotic atoms\footnote{Here the long-range interaction is the attractive Coulomb force. The so-called Deser-Trueman formula \cite{39} relates exotic atom’s energy levels to the short-distance interaction’s scattering length.} and quantum dots [39].

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\[\text{[9]}\ S. Elhatisari, D. Lee, G. Rupak, E. Epelbaum, H. Krebs, T. A. Lhde, T. Luu, and U.-G. Meiner, \textit{Nature} \textbf{528}, 111 (2015), arXiv:1506.03513 [nucl-th].\]
SUPPLEMENTAL MATERIAL

An exactly solvable case: hard-sphere potential

We demonstrate here that if the interaction is short-ranged and has the form of a hard sphere, the solution to Eq. (2) can be found analytically. This model was studied in Ref. [13] by using parabolic cylinder functions for s-wave channel. We define the hard-sphere potential as \( V_s(r) = \infty \) if \( r \leq r_c \) and 0 otherwise \( (r \equiv |r| \) with \( r \) the relative displacement between the two particles). In addition, each particle experiences an external harmonic potential. Because the CM motion is factorized, we just focus on the relative motion; the corresponding external potential is \( M_n \omega^2 r^2/2 \), with \( M_n \) the reduced mass.

Let us define \( \bar{r} \equiv r/b \) and \( \bar{r}_c \equiv r_c/b \) with \( b \equiv 1/\sqrt{M_n \omega} \), and \( \bar{E} \equiv E/\omega \). When \( \bar{r} > \bar{r}_c \), the Schrödinger equation in the \( \ell \)th partial wave becomes

\[
\left[ -\frac{d^2}{dr^2} + \frac{\ell (\ell + 1)}{r^2} + \bar{r}^2 \right] u_\ell = 2 \bar{E} u_\ell ,
\]

with the radial wave function defined as \( u_\ell(\bar{r})/\bar{r} \). Thus, the wave function at \( \bar{r} > \bar{r}_c \) is a linear combination of two independent solutions to the harmonic oscillator Schrödinger equation [17]:

\[
u_\ell = e^{-\bar{r}^2/2} \left[ c_1 \bar{r}^{\ell+1} M \left( \frac{\ell}{2} + \frac{3}{4}, \ell + \frac{3}{2}, \bar{r}^2 \right) \right. \\
\left. + c_2 \bar{r}^{-\ell} M \left( -\frac{\ell}{2} + \frac{1}{4}, -\ell + \frac{1}{2}, \bar{r}^2 \right) \right] ,
\]

where \( M(a,b,z) \) is the Kummer function [40].

When \( \bar{r} \to +\infty \), \( u_\ell \) should go to zero to guarantee that the wave function is normalized. Since at large \( z \) [37, Eq. 13.7.2]

\[
M(a,b,z) \approx \Gamma(b) \left[ z^{a-b} e^z \right. \\
\left. \frac{(-z)^{-a}}{\Gamma(a)} \right] \left[ 1 + O(z^{-1}) \right],
\]

we require

\[
c_1 \frac{\Gamma(\ell + \frac{3}{2})}{\Gamma\left( \frac{\ell}{2} + \frac{3}{4} - \frac{\bar{E}}{2} \right)} + c_2 \frac{\Gamma(-\ell + \frac{1}{2})}{\Gamma\left( -\frac{\ell}{2} + \frac{1}{4} - \frac{\bar{E}}{2} \right)} = 0 .
\]

Meanwhile, \( u_\ell(\bar{r}_c) = 0 \) implies

\[
\left. c_1 \bar{r}_c^{\ell+1} M \left( \frac{\ell}{2} + \frac{3}{4} - \frac{\bar{E}}{2}, \ell + \frac{3}{2}, \bar{r}_c^2 \right) \right. \\
\left. + c_2 \frac{\bar{r}_c^{-\ell}}{\bar{r}_c^2} M \left( -\frac{\ell}{2} + \frac{1}{4} - \frac{\bar{E}}{2}, -\ell + \frac{1}{2}, \bar{r}_c^2 \right) \right] = 0 .
\]

Equations (20)–(21) have nontrivial solutions only if the corresponding determinant is zero, which gives the quantization condition:

\[
\frac{(2\bar{r}_c)^{2\ell+1}}{(-)^\ell} \frac{\Gamma\left( \frac{\ell}{2} + \frac{3}{4} - \frac{\bar{E}}{2} \right)}{\Gamma\left( \frac{1}{2} - \frac{\ell}{2} - \frac{\bar{E}}{2} \right)} M \left( \frac{1}{4}, \frac{\ell}{2} + \frac{3}{4} - \frac{\bar{E}}{2}, \ell, \bar{r}_c^2 \right) = M \left( \frac{1}{4}, \frac{\ell}{2} - \frac{\bar{E}}{2}, \ell, \bar{r}_c^2 \right) .
\]
Here, \( \mathcal{N}_\ell \equiv (2\ell + 1)!(2\ell - 1)! \left[ (-1)^\ell \right] \equiv 1 \).

Note that the left side of Eq. (22) is the right side of Eq. (1) multiplied by a \( (-1)^{2\ell+1}/\mathcal{N}_\ell \) factor. Meanwhile, the phase shift due to \( V_c(r) \) in the \( \ell \)th partial wave is tan \( \delta_\ell = j_\ell(p_r)/y_\ell(p_r) \) [41]. Thus the deficiency of Eq. (1) is identified as the difference between the left side of Eq. (1) multiplied by \( -r_c^{-2\ell+1}/\mathcal{N}_\ell \) and the right side of Eq. (22), i.e.,

\[
\frac{(pr_c)^{2\ell+1}}{(-)\mathcal{N}_\ell \ j(p_r)} \frac{y_\ell(pr_c)}{y_\ell(p_r)} = \frac{M \left( \frac{1}{2} - \frac{\ell}{2} - \frac{\bar{E}}{2} \right)}{M \left( \frac{1}{2} + \frac{\ell}{2} + \frac{\bar{E}}{2} \right)}.
\]

(23)

The left side can be expanded in terms of \((pr_c)^2\) :

\[
1 + \frac{(2\ell + 1)(pr_c)^2}{4\ell(\ell + 1) - 3} + \frac{(\ell + 3)(2\ell + 1)(pr_c)^4}{(2\ell - 3)(2\ell - 3)\ell^2(2\ell + 5)} + \cdots
\]

(24)

Now according to Ref. [37, Eq. (13.2.2)], \( M(a, b, z) \) can be expanded as \( 1 + \frac{a}{z} + \frac{a(a + 1)z^2}{2!} + \cdots \), indicating that Eq. (23)’s right side, a function of \( E \) and \( r_c \), can be approximated by a double expansion in terms of powers of \( \bar{r}_c^2 \) and \( 2\bar{E}\bar{r}_c^2 \) when both are small (note that the coefficient denominators in the expansion of the \( M \) functions in Eq. (23) are independent of \( E \) and \( r_c \)). This also suggests the difference between left and right sides in Eq. (23) can be expanded in terms of \( \bar{r}_c^2 \) and \( 2\bar{E}\bar{r}_c^2 \).

It can be shown that with \( \omega \to 0 \) and \( \bar{E} \) and \( r_c \) fixed, the right side of Eq. (23) approaches its left side. In this limit, \( \bar{E} \to \infty \),

\[
\lim_{\omega \to 0} \frac{M \left( -\frac{\ell}{2} - \frac{1}{4} - \frac{\bar{E}}{2} - \ell + \frac{1}{2} \bar{r}_c^2 \right)}{M(\omega)} = \lim \frac{M \left( -\frac{\ell}{2\omega} - \ell + \frac{1}{2} \bar{r}_c^2 M_\omega \right)}{M(\omega)} = a_0 \frac{F_1 \left( \ell + \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2} \right)}{M_\omega \bar{r}_c^2 M_\omega},
\]

(25)

The following expansion is expected, with the first two terms explicitly given:

\[
\frac{(-1)^{\ell+1} 2\bar{r}_c}{b} \frac{(pr_c)^{2\ell+1}}{\mathcal{N}_\ell} \frac{\Gamma \left( 4 - \ell - 2 \bar{E} \right)}{\Gamma \left( 4 - \ell - 2 \bar{E} \right)} - \frac{(pr_c)^{2\ell+1}}{\mathcal{N}_\ell} \cot \delta_\ell(p) = \frac{(2\ell + 1)}{2(2\ell - 3)(2\ell + 5)} \frac{(pr_c)^{2\ell+1}}{\mathcal{N}_\ell} \cot \delta_\ell(p) + \cdots
\]

(26)

Meanwhile, the ERE for \( V_c \) can be derived easily from Eq. (24): \( (pr_c)^{2\ell+1} \cot \delta_\ell(p) / \mathcal{N}_\ell = \sum_{i=j=0}^{\infty} C_{i,j} \Gamma \left( \frac{1}{2} + \frac{2i - 1}{4} \right) (pr_c)^{2j} \).

If a high-momentum scale \( M_\mu = r_c^{-1} \) is identified, Eq. (30) can be transformed to Eq. (2) after redefining \( C_{i,j} = \mathcal{N}_\ell M_\mu^{2\ell+1-4i-2j} \mathcal{C}_{i,j} \).

The 2nd model for numerical testing

Here a simple square-well model [25] is used to test the improved BERW formula. The potential was constructed to qualitatively describe neutron-\( \alpha \) scattering in the s- and p-waves [25]. The quantum numbers for the considered channels in \( J^\pi \) notation are \( \frac{1}{2}^+ \), \( \frac{1}{2}^- \) and

FIG. 2. The neutron-\( \alpha \) s-wave and p-wave scattering phase shifts vs. their CM energy \( E \), as produced by a model square-well potential (see text) [25].
- The potential $V_\alpha(r) = V_0(1 + \beta \mathbf{L} \cdot \mathbf{\sigma})$ when $r < r_c$ and 0 when $r > r_c$, with $V_0 = -33$ MeV, $r_c = 2.55$ fm, $\beta = 0.103$ [25]. $\mathbf{L} \cdot \mathbf{\sigma}$ is the spin-orbit coupling, which generates differences between the $p_{3/2}$ and $p_{1/2}$ channels.

In this exercise, the potential is treated as the exact underlying physics for the two particles. The phase shifts, calculated by solving the corresponding Schrödinger equations in the continuum, are shown in Fig. 2. These phase shifts are considered to be “exact” ones. (The $s_{3/2}$ channel’s exact phase shift is also shown in Fig. 1.) Meanwhile, the spectra for the two particles in various harmonic potential traps can also be precisely computed. The goal is to test the original and the improved BERW formulas using these exact phase shifts and energy spectra.

In Fig. 3, the discrete symbols are the differences between the two sides in Eq. (1) divided by $M_{H}^{2\ell+1}$ at eigenenergies associated with the trap frequency $\omega = 0.1$, $\sqrt{0.1}$, 1, $\sqrt{10}$ and 10 MeV. We take $M_{H} = 200$ MeV ($\sim 1$ fm$^{-1}$), as motivated by the value of $r_c$. We can see that the leading-order difference does scale as $\omega^2$.

Also, in the s-wave channel there is a deep bound state in free space—unphysical for the n-α system—and thus a distinct negative eigenenergy in all the traps. However, for the other two channels no bound state exists in free space.

To see how well the improved BERW formula works, we need to know the values of $C_{i,j}$ corresponding to this particular potential. First, another set of eigenenergies at extremely small trap frequencies (both on the order of $10^{-6}$ MeV) is computed. Second, they are used as inputs to fit $C_{i,j}$ values based on the improved BERW formula. A least-squares fit uses as the objective function the sum of the squares of the differences between the two sides in Eq. (2), as calculated at those small eigenenergies. The small values of $\omega$ and eigenenergies help separate the impact of $C_{i,j}$ at different orders, and enables a precise fit (it amounts to computing derivatives at $E = 0$ and $\omega = 0$ with points separated by tiny distances). The series in Eq. (2) is nonetheless truncated to $i \leq 2$ and $j \leq 3$. To make the parameters dimensionless, we can rescale them by appropriate powers of $M_{H}$. $C_{i,j} \equiv \overline{C}_{i,j} M_{H}^{2\ell+1-4i-2j}$. The best-fit values for $\overline{C}_{i,j}$ are shown in Tables I, II, and III.

A few higher-order $\overline{C}_{i,j}=2$ values are not shown in those tables, because over-fitting [43] in this simple exercise leads to values significantly larger than 1. However, these contributions are very small in the plots shown if they on the order of 1 (their natural size), and therefore they are set to zero in generating the plots.

### Table I. $\overline{C}_{i,j}$ for the $s_{1/2}$ channel.

| $i$ | 0      | 1      | 2      |
|-----|--------|--------|--------|
| 1   | 0.3536 | -0.4097| 0.004206 |
| 2   | 0.7898 | -0.1756| -0.4063  |
| 3   | -0.01278 | 0.2949 |

### Table II. $\overline{C}_{i,j}$ for the $p_{3/2}$ channel.

| $i$ | 0      | 1      | 2      |
|-----|--------|--------|--------|
| 1   | 0.2304 | -1.870 | 0.5400  |
| 2   | -0.5571 | -0.8676| 0.3118  |
| 3   | 0.5609 | -0.2829|        |

### Table III. $\overline{C}_{i,j}$ for the $p_{1/2}$ channel.

| $i$ | 0      | 1      | 2      |
|-----|--------|--------|--------|
| 1   | 0.1390 | -2.084 | 0.7400  |
| 2   | -0.4427 | -1.090 | 0.5210  |
| 3   | 0.6225 | -0.4064|        |
Having determined the $C_{i,j}$, the $C_{i\neq 0,j}$ terms in Eq. (2) are used in Fig. 3 to interpolate between the discrete symbols, i.e., the difference between the right and left sides of Eq. (1) as computed at discrete eigenenergies up to $\approx 20$ MeV. Because the fitting of $C_{i,j}$ is carried for $E$ and $\omega$ near zero ($\sim 10^{-6}$ MeV), the agreement with the interpolating functions demonstrates that the deficiency of Eq. (1) can indeed be expanded in powers of $\omega^2$ and $p^2$, as implied by the improved BERW formula in Eq. (2).

A proof of Eq. (16)

![Fig. 4. The contours for the integration in the complex $\tilde{u}$ plane.](image)

Let us redefine $\tilde{z} \equiv z - \ell/2 - 3/4$, and

\[
\hat{f}_\ell(\tilde{z}, n) \equiv f_\ell(\tilde{z} + \ell/4, n) = \frac{\Gamma(n + \ell + 3/2)}{\Gamma(n + 1)} (\tilde{z} - n),
\]

\[
g_\ell(\tilde{z}) \equiv (-)^\ell \pi \frac{\Gamma(-\tilde{z})}{\Gamma(-\ell - 1/2 - \tilde{z})}.
\]

Equation (16) then becomes

\[
\sum_{n=0}^{\infty} \hat{f}_\ell(\tilde{z}, n) = g_\ell(\tilde{z}).
\]

The renormalization $\mathcal{F}$ is defined by Eq. (10) and the relationship between $T_A$ and $n_A$ that guarantees the cancelation of the divergences on that equation’s left side. The proof starts with integrating $g_\ell(\tilde{u})/(\tilde{u} - \tilde{z})$ in the complex $\tilde{u}$ plane over a large contour around the origin and crossing between the two singularities at $\tilde{u} = n_A$ and $n_A + 1$ on the positive real axis. The contour $C_r + C_\epsilon$ is plotted in Fig. 4. After rearranging terms we have

\[
g_\ell(\tilde{z}) = \sum_{n=0}^{n_A} \hat{f}_\ell(\tilde{z}, n) + \frac{1}{2\pi i} \oint_{C_r+C_\epsilon} d\tilde{u} \frac{g_\ell(\tilde{u})}{\tilde{u} - \tilde{z}}.
\]

The left side comes from the residue of the $1/(\tilde{u} - \tilde{z})$ pole in the contour integration while the series sum on the right side is from the residues of $g_\ell(\tilde{u})$’s poles (all on the positive real axis) in the same integration. Comparing Eq. (34) to Eq. (33) suggests that the contour integration in Eq. (34) should cancel the series’s divergence as the $\tilde{T}_\Lambda$ terms—i.e., those from $\mathcal{F} \Sigma(E)$—do in Eq. (10). This is the focus of the following proof.

As preparation, it is important to understand the behavior of $g_\ell(\tilde{u})$ in two different regions (define $\theta_0 \equiv \arg(\tilde{u})$ and $R$ as the radius of $C_r$): $\pi \geq |\theta_0| \gg R^{-1}$ and $|\theta_0| \lesssim R^{-1}$. Let us look at the region close to the positive real axis first. Considering the presence of $g_\ell(\tilde{u})$’s poles, it is easier to use the following re-expression based on $\{37, Eq. 5.5.3\}$:

\[
g_\ell(\tilde{u}) = \pi \cot(\pi \tilde{u}) \frac{\Gamma(\ell + \frac{3}{2} + \tilde{u})}{\Gamma(1 + \tilde{u})}.
\]

This expression moves the poles from the $\Gamma$ function to the cot function. When $R \to +\infty$,

\[
cot(\pi \tilde{u}) = \begin{cases} e^{i\pi \tilde{u}} + e^{-i\pi \tilde{u}} & \text{if } \tilde{u} > 0 \\ e^{i\pi \tilde{u}} - e^{-i\pi \tilde{u}} & \text{if } \tilde{u} < 0 \end{cases} \approx \frac{1}{\tilde{u}}.
\]

Here $\theta_0$ is a small positive number. Therefore, $\cot(\pi \tilde{u}) \sim -i \text{sgn}(\text{Im } \tilde{u})$ when $\pi - \theta_0 > |\theta_0| \gg R^{-1}$ [the error scales as $\exp(-2\pi |\text{Im } \tilde{u}|)$], but in the 2nd region, $|\theta_0| \lesssim R^{-1}$, and its behavior is qualitatively different.

Since the $\Gamma$ function ratio in Eq. (35) is the same as that ratio in $\tilde{f}_\ell(\tilde{z}, n)$ with $n \to \tilde{u}$, by applying the asymptotic expansion from Eq. (11) on the right side of Eq. (35), we get, when $R \to +\infty$ such that $R \gg |\tilde{z}|$ and $\pi - \theta_0 > |\theta_0| \gg R^{-1}$,

\[
g_\ell(\tilde{u}) \sim -i\pi \text{sgn}(\text{Im } \tilde{u}) \left( \sum_{k=0}^{\infty} G_k (\ell + \frac{3}{2} + 1) \right) \frac{\tilde{z}^{k'}}{\tilde{u}^{k'+1}}.
\]

Here $\tilde{f}_\ell(\tilde{z}, \tilde{u})$ is the asymptotic expansion of $\hat{f}_\ell(\tilde{z}, \tilde{u})$ in terms of $1/\tilde{u}$ using Eq. (11). It turns out the above expansion also holds when $\theta_0 \to \pi$ or $-\pi$. However, using Eq. (35) to understand $g_\ell$ close to the negative real axis is awkward, as it involves the cancelation of poles from the cot and the $\Gamma$ functions. Instead, Eq. (11) can be applied to analyze the original form of $g_\ell(\tilde{u})$ (see Eq. (32)):

\[
g_\ell(\tilde{u}) \sim (-)^\ell \pi (-\tilde{u})^{\ell/2 + \frac{1}{2}} \sum_{k=0}^{\infty} G_k \frac{0, -\ell - \frac{1}{2}}{(-\tilde{u})^k}
\]

\[
= -i \text{sgn}(\text{Im } \tilde{u}) \pi \tilde{u}^{\ell+\frac{1}{2}} \sum_{k=0}^{\infty} G_k (\ell + \frac{3}{2} + 1) \frac{\tilde{z}^{k'}}{\tilde{u}^{k'+1}}.
\]
Here \( G_k(\ell + \frac{3}{2}, 1) = (-)^k G_k(0, -\ell - \frac{1}{2}) \) is used, which can be inferred from its definition [37, Eq. 5.11.17] [38] and properties of the generalized Bernoulli polynomials. It is worth pointing out that the \( \text{sgn}(\text{Im} \hat{u}) \) factor moves the asymptotic series’s branch cut on the negative real axis due to the \( \sqrt{\pi} \) factor to the positive real axis, ensuring that the expansion series is analytic around the negative real axis. Therefore, Eq. (37) holds when \( \pi \geq |\theta_u| \gg R^{-1} \), but not in the \( |\theta_u| \lesssim R^{-1} \) region. This suggests splitting the contour integration into two major pieces:

\[
\int_{C_e + C_e - S} \frac{i\pi \text{sgn}(\text{Im} \hat{u}) f^E_{\ell}(\bar{z}, \hat{u})}{2\pi i} d\hat{u}
\]

\( 1^{st} \) piece

\[
+ \int_{C_e + C_e - S} \frac{d\hat{u}}{2\pi i} \left[ \frac{g_u(\hat{u})}{\hat{u} - \bar{z}} - i\pi \text{sgn}(\text{Im} \hat{u}) f^E_{\ell}(\bar{z}, \hat{u}) \right].
\]

\( 2^{nd} \) piece

In \( C_e + C_e - S \), \( S \) is the point where \( C_e \) crosses the real axis. Thus the contour means to integrate infinitely close to the upper and lower real axis, because of the corresponding integrand’s branch cut on the positive real axis. In the \( 2^{nd} \) piece, the first term should be integrated over \( C_e + C_e \). However, since the integrand is continuous across the point \( S \) as long as \( \epsilon \neq 0 \), changing the contour to \( C_e + C_e - S \) does not affect the results.

Integrating the \( 1^{st} \) piece over \( C_e \) with \( \epsilon \to 0^+ \) gives

\[
\int_{0<\theta_u<2\pi} \frac{d\bar{z}}{\sqrt{\pi}} = \int_{0<\theta_u<\pi} dv \frac{u^{2j}}{\partial^n u^{2j-1}} B_{2j}.
\]

Here \( f^E_{\ell}(\hat{z}, \hat{u}) \) truncates the expansion in \( f^E_{\ell}(\hat{z}, \hat{u}) \) by only keeping terms with powers of \( \hat{u} \) from \( \ell - 1/2 \) to \(-1/2\) (the neglected terms’ integration vanishes no slower than \( 1/\sqrt{R} \) as \( R \to \infty \)). In the derivation, (1) the \(-\pi \leq \theta_u < 0 \) branch has been rotated by \( +2\pi \), which eliminated the \( \text{sgn}(\text{Im} \hat{u}) \) factor because of the \( \sqrt{\pi} \) factor in the integrand; (2) a transformation, \( \hat{u} = v^2 \), was used; and (3) the fact that \( v f^E_{\ell}(\hat{z}, v^2) \) is analytic in the upper complex \( v \) plane and an even function on the real axis was used. Note that integrating the \( 1^{st} \) piece over \( C_e - S \) gives 0 with \( \epsilon \to 0^+ \).

For the \( 2^{nd} \) piece, the \( C_e + C_e - S \) contour can be deformed to \( C_L + C_R - C_e + C_{R+} - S \) without crossing any singularities, with the left and right segments connecting at \( \infty \). The integrand on the two sets of contours (including in the area enclosed by them) is 0 up to at most a \( \sim e^{-R\#} \) correction (with \( \# \) as a positive number), except on the segments with \( |\theta_u| \lesssim 1/R \) along \( C_{R\pm} \) and \( C_e \). Therefore, \( C_L \) can be safely ignored. Let us focus on \( C_R - C_e + C_{R+} - S \). Since

\[
\frac{g_u(\bar{u})}{\bar{u} - \bar{z}} \sim -\pi \cot(\pi \bar{u}) f^E_{\ell}(\bar{z}, \bar{u}),
\]

the \( 2^{nd} \) piece is

\[
\int_{C_R \pm + C_e - S} \frac{d\hat{u}}{2\pi i} (\pi \cot(\pi \bar{u}) + i \text{sgn}(\text{Im} \hat{u})) f^E_{\ell}(\bar{z}, \hat{u}) \).
\]

Note that \( \cot(\pi \bar{u}) \sim 1/[(\bar{u} - n\Lambda)] \) when \( \bar{u} \to n\Lambda \), its integration over \( C_e - S \) with \( \epsilon \to 0^+ \) gives \( -(\bar{f}^E_{\ell}(\bar{z}, n\Lambda))/2 \).

Integrating over \( C_{R\pm} \) with \( \epsilon \to 0^+ \) gives

\[
\int_{\epsilon}^{+\infty} \frac{d\bar{z}}{2\pi i} \frac{\bar{f}^E_{\ell}(\bar{z}, n\Lambda + i\Delta)}{e^{2\pi\Delta} - 1} - \int_{-\infty}^{-\epsilon} \frac{d\bar{z}}{2\pi i} \frac{\bar{f}^E_{\ell}(\bar{z}, n\Lambda + i\Delta)}{e^{-2\pi\Delta} - 1} = \int_{0}^{+\infty} \frac{d\bar{z}}{2\pi i} \frac{\bar{f}^E_{\ell}(\bar{z}, n\Lambda - i\Delta)}{e^{2\pi\Delta} - 1}.
\]

Because the integration is dominated by the \( \Delta \ll n\Lambda \) region, the two \( \bar{f}^E_{\ell} \) are expanded in terms of Taylor series for the \( 2^{nd} \) argument at \( n\Lambda \) in the above derivation. The resulting integrations are proportional to Riemann \( \zeta(2j) \) at even arguments, which are related to Bernoulli numbers [37, Eq. 25.5.1, 25.6.2, 24.2.2]. Adding all the contributions, we can see that the \( 2^{nd} \) term on the right side of Eq. (34) can be approximated by

\[
\sum_{j=1}^{n\Lambda} \frac{\partial^{2j-1} \bar{f}^E_{\ell}(\bar{z}, n\Lambda)}{(2j)!} B_{2j},
\]

with the error scaling as \( e^{-n\Lambda\#} \) (\( \# \) is a positive constant).

This expression is exactly the same as the divergent \( n\Lambda \)-dependent pieces in \( \Sigma_{\infty} \)'s series sum derived using Eq. (12), which completes the proof.

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2 As usual [37, Eq. 1.9.7], the \( \sqrt{\pi} \) branch cut in the complex \( \hat{u} \) plane is on the negative real axis. Meanwhile \( \Sigma(E) \) (and the related scattering \( T \)-matrix), as calculated in Eq. (5), in the complex \( E \) plane has a branch cut separating physical and unphysical sheets on the positive real axis [44], because it involves \(-ip = \sqrt{(2M_R E + \Delta^2)}\).