Toward extracting scattering phase shifts from integrated correlation functions. IV. Coulomb corrections

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The formalism developed in Guo and Gasparian [Toward extracting the scattering phase shift from integrated correlation functions, Phys. Rev. D **108**, 074504 (2023)]; Guo [Toward extracting the scattering phase shift from integrated correlation functions. II. A relativistic lattice field theory model, Phys. Rev. D **110**, 014504 (2024)]; and Guo and Lee [Toward extracting scattering phase shift from integrated correlation functions. III. Coupled channels, Phys. Rev. D **111**, 054506 (2025)] that relates the integrated correlation functions for a trapped system to the infinite volume scattering phase shifts through a weighted integral is further extended to include Coulomb interaction between charged particles. The original formalism cannot be applied due to different divergent asymptotic behavior resulting from the long-range nature of the Coulomb force. We show that a modified formula in which the difference of integrated correlation functions between particles interacting with Coulomb plus short-range interaction and with Coulomb interaction alone is free of divergence, and has rapid approach to its infinite volume limit. Using an exactly solvable model, we demonstrate that the short-range potential scattering phase shifts can be reliably extracted from the formula in the presence of Coulomb interaction.

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I. INTRODUCTION

Scattering plays a crucial role in a wide range of dynamics, from the strong interaction in quantum chromodynamics (QCD) to atomic interactions in condensed matter physics. Precisie determination of scattering amplitudes in such systems remains fundamental but challenging. In most cases, numerical simulations based on stochastic evaluation of the path integral are performed by placing the system in artificial traps, such as a periodic finite box or a harmonic oscillator trap. The traps lead to quantized energies in the system, which are then connected to the infinite volume scattering amplitudes through quantization conditions, such as the Lüscher formula [1] for periodic boxes, and Busch-Englert-Rzażewski-Wilkens (BERW) formula [2] in harmonic oscillator traps. A lot of progress has been made in recent years on extracting multihadron dynamics in nuclear physics, where a Lüscher- or BERW-like formula has been successfully extended into inelastic channel, three-body channel, and other systems, see, e.g., Refs. [3–42]. In addition to the Lüscher-like method, there is the Hadrons to Atomic nuclei from Lattice QCD potential method [43–47] that also relies on the discrete energy spectrum.

In multinucleon systems, issues such as the signal-to-noise (S/N) ratio of lattice correlation functions [48,49] and the requirement of increasingly large number of interpolating operators at large volumes [50], present unique challenges to Lüscher-like methods. These challenges motivated alternative approaches. To this end, the integrated correlation function method was proposed recently in Ref. [51]. It relates the difference between interacting and noninteracting integrated correlation functions of two nonrelativistic particles in an artificial trap to the infinite-volume phase shift through a weighted integral. The main advantage of the method is working directly with correlation functions, bypassing the energy spectrum determination. Furthermore, the relation has a rapid convergence rate at short Euclidean times, even with a modestly small sized trap [51]. This makes it potentially a good candidate to overcome the S/N problem in multinucleon systems.

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The formalism is by construction free from issues encountered at large volumes, such as increasingly dense energy spectrum and the extraction of low-lying states. The integrated correlation function formalism was later extended to include relativistic dynamics [52], coupled channel effects in [53,54], and its potential simulation on quantum computers [55].

The aim of the present work is to further develop the integrated correlation function formalism to include long-range Coulomb interaction between charged particles, in conjunction with short-range interactions. It is a necessary step to describe charged-hadron interactions in nuclear physics and lattice QCD. Coulomb corrections have been considered in traditional formalisms in harmonic traps [56–58], and periodic boxes [59–62].

In the integrated correlation function formalism considered here, due to the distortion of long-range Coulomb interaction on the asymptotic wavefunction, the Coulomb-modified integrated correlation function has a different divergent asymptotic behavior from that of the noninteracting integrated correlation function. Consequently, the difference between the Coulomb-modified integrated correlation function and the noninteracting integrated correlation function in the original formalism is cutoff dependent and divergent, rendering it inapplicable to scattering problems with Coulomb interaction. We will show that the issue can be resolved by carefully incorporating the asymptotic behavior of the correlation function due to pure Coulomb interaction.

The paper is organized as follows. A brief summary of integrated correlation function formalism is outlined in Sec. II. The extension to Coulomb interaction is presented in Sec. III. A numerical test with an exactly solvable contact interaction in a spherical hard-wall trap is discussed in Sec. IV, followed by summary and outlook in Sec. V. Some technical details are in two Appendixes.

II. INTEGRATED CORRELATION FUNCTION FORMALISM WITHOUT COULOMB INTERACTION

In this section, we outline the essential ingredients of the integrated correlation function formalism needed in the discussion of Coulomb interaction in the next section.

A relation in $1+1$ dimensional spacetime that connects the integrated correlation functions for two nonrelativistic particles in a trap to the scattering phase shift due to a short-range interaction potential, $\delta(\epsilon)$, through a weighted integral, was derived in Ref. [51],

$$C(t) - C^{(0)}(t) \overset{\text{trap}\to\infty}{\longrightarrow} \frac{1}{\pi}\int_0^\infty d\epsilon \frac{d\delta(\epsilon)}{d\epsilon} e^{-i\epsilon t} + \frac{\delta(0)}{\pi}, \quad (1)$$

where $C(t)$ and $C^{(0)}(t)$ are Minkowski time integrated correlation functions for two interacting and noninteracting particles in the trap.

The $3+1$ dimensional spacetime extension of Eq. (1) is given in Eq. (13) by, see derivations below,

$$C_l(t) - C_l^{(0)}(t) \overset{\text{trap}\to\infty}{\longrightarrow} (2l+1)\frac{it}{\pi}\int_0^\infty d\epsilon \delta_l^{(S)}(\epsilon) e^{-i\epsilon t}, \quad (2)$$

where $C_l(t)$ and $C_l^{(0)}(t)$ are partial-wave-projected integrated correlation functions of angular momentum l, and $\delta_l^{(S)}(\epsilon)$ stands for the l-th partial-wave scattering phase shift due to a short-range interaction potential (emphasized by the superscript S). We also assume that $\delta_l^{(S)}(0) = 0$. The extra factor $(2l+1)$ is the result of partial-wave projection. We remark that at current scope of presentation, we will limit ourself to the traps that preserve rotational symmetry, such as harmonic oscillator trap and spherical hard-wall trap, so that angular momenta are good quantum numbers. The partial-wave expansion of trapped wavefunction and Green's function depends only on orbital quantum number-l, not magnetic quantum number-m_l where $m_l \in [-l, \ldots, l]$. In cases where continuous rotational symmetry is no longer the symmetry group of the trap, such as a periodic cubic box, the dynamic equations of a trapped system have to be projected into the irreducible representations (irreps) of the cubic symmetry group. The projection of each irrep of the cubic symmetry group typically involves the mixture of angular momentum partial waves, see, e.g., [16,63]. Typically the higher angular momentum components could be neglected due to the threshold barrier factor suppression at low energy and exponential factor in the integrand of the Euclidean time, and irrep projection is dominated by the few lowest angular momentum components. Similar effects are expected in the integrated correlation function approach. On top of that, due to the suppression of the extra relativistic kinematic factor and exponential decaying factor in the Euclidean time, see, e.g., Ref. [52], the inifinite volume limit of the difference of integrated correlation functions should still be dominated by low-energy dynamics. We leave the technical aspects of irreps projection for periodic box traps for future discussion.

The integrated forward time propagating two-particle correlation function for nonrelativistic systems is defined through summing over all the modes of two-particle correlation functions along the diagonal,

$$C_l(t) = (2l+1)\int_0^\infty r^2 dr \langle 0|\hat{\mathcal{O}}_l(r,t)\hat{\mathcal{O}}_l^\dagger(r,0)|0\rangle. \quad (3)$$

The $\hat{\mathcal{O}}_l^\dagger(r,0)$ and $\hat{\mathcal{O}}_l(r,t)$ denote creation and annihilation operators to create two particles with relative radial coordinate r and angular momentum l at time 0 at the source, and then to annihilate them with relative radial coordinate of r at later time t at the sink, respectively. Examples of construction of two-particle creation operators

in 1 + 1 dimensions can be found in Eq. (5) in Ref. [53], or Eq. (4) in Ref. [55].

We also showed in Ref. [51] that two-particle correlation functions can be expressed in terms of wavefunctions in the spectral representation. By inserting a complete energy basis in between two-particle creation and annihilation operators, $\sum_\epsilon |\epsilon\rangle\langle\epsilon| = 1$, the wavefunction defined via,

$$\langle\epsilon|\hat{\mathcal{O}}_l^\dagger(r,0)|0\rangle = \psi_l^*(r;\epsilon), \tag{4}$$

satisfies the radial Schrödinger equation for a trapped system (we use a dimensionless unit system in which $\hbar = c = 1$),

$$\left[-\frac{1}{2\mu r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{l(l+1)}{2\mu r^2} + U_{trap}(r) + V(r)\right]\psi_l(r;\epsilon) = \epsilon\psi_l(r;\epsilon), \tag{5}$$

where μ denotes the reduced mass of the two-particle system, and $U_{trap}(r)$ and $V(r) = V_S(r)$ are trap potential and short-range two-particle interaction potential, respectively. Thus in spectral representation the integrated nonrelativistic two-particle correlation function is given by [51],

$$C_l(t) = (2l+1)\int_0^\infty r^2 dr \sum_\epsilon \psi_l(r;\epsilon)\psi_l^*(r;\epsilon)e^{-i\epsilon t}. \tag{6}$$

A relatively simple way to show the connection between Eqs. (2) and (6) is to consider the asymptotic behavior of infinite-volume wavefunctions,

$$\psi_l^{(\infty)}(r;\epsilon) \xrightarrow{r\to\infty} \frac{4\pi i^l}{kr}\sin\left(kr - \frac{\pi l}{2} + \delta_l^{(S)}(\epsilon)\right), \tag{7}$$

where $k = \sqrt{2\mu\epsilon}$ is the relative momentum in the center of mass. Using the identity relation [see Eq. (31) of Ref. [64]] involving the radial wavefunction,

$$2k\int_0^\Lambda dr\left|u_l^{(\infty)}(r;k)\right|^2 = \partial_\Lambda u_l^{(\infty)*}(\Lambda;k)\partial_k u_l^{(\infty)}(\Lambda;k) - u_l^{(\infty)*}(\Lambda;k)\partial_k\partial_\Lambda u_l^{(\infty)}(\Lambda;k), \tag{8}$$

where $\Lambda \to \infty$ is a distance that is far larger than the potential range, and its relation to the asymptotic form in Eq. (7),

$$u_l^{(\infty)}(r;k) = \frac{kr}{4\pi i^l}\psi_l^{(\infty)}(r;\epsilon), \tag{9}$$

we find that

$$\int_0^\Lambda dr\left|u_l^{(\infty)}(r;k)\right|^2 \xrightarrow{\Lambda\to\infty} \frac{\Lambda}{2} + \frac{\sin(2k\Lambda - \pi l)}{4k} + \frac{1}{2}\frac{d\delta_l^{(S)}(\epsilon)}{dk}. \tag{10}$$

Its corresponding noninteracting form is given by,

$$\int_0^\Lambda dr\left|u_l^{(0,\infty)}(r;k)\right|^2 \xrightarrow{\Lambda\to\infty} \frac{\Lambda}{2} + \frac{\sin(2k\Lambda - \pi l)}{4k}. \tag{11}$$

We see that Eqs. (10) and (11) have the same divergent asymptotic terms, and they cancel out in the difference,

$$\int_0^\Lambda dr\left[\left|u_l^{(\infty)}(r;k)\right|^2 - \left|u_l^{(0,\infty)}(r;k)\right|^2\right] \xrightarrow{\Lambda\to\infty} \frac{1}{2}\frac{d\delta_l^{(S)}(\epsilon)}{dk}, \tag{12}$$

which remains finite and is free of the integration cutoff Λ. Therefore, at infinite volume limit, the difference of integrated correlation functions between interacting and noninteracting cases takes the form,

$$\begin{aligned} C_l(t) - C_l^{(0)}(t) &\xrightarrow{\text{trap}\to\infty} (2l+1)\int_0^\infty \frac{k^2 dk}{(2\pi)^3} \\ &\times \frac{(4\pi)^2}{k^2}\int_0^\Lambda dr\left[\left|u_l^{(\infty)}(r;k)\right|^2 - \left|u_l^{(0,\infty)}(r;k)\right|^2\right]e^{-i\frac{k^2}{2\mu}t} \\ &\xrightarrow{\Lambda\to\infty} \frac{(2l+1)}{\pi}\int_0^\infty d\epsilon\frac{d\delta_l^{(S)}(\epsilon)}{d\epsilon}e^{-i\epsilon t}, \end{aligned} \tag{13}$$

which yields Eq. (2) after integration by part.

A more rigorous way of proving Eq. (2) is to use the Green's function representation of integrated correlation functions, see technical details in Refs. [51,53],

$$C_l(t) = i\int_{-\infty}^\infty \frac{d\lambda}{2\pi}\mathrm{Tr}\left[G_l^{(trap)}(\lambda)\right]e^{-i\lambda t}. \tag{14}$$

The partial-wave Green's function $G_l^{(trap)}$ is the solution of partial-wave Dyson equation, whose spectral representation is given by,

$$G_l^{(trap)}(r,r';\lambda) = \sum_\epsilon \frac{\psi_l(r;\epsilon)\psi_l^*(r';\epsilon)}{\lambda - \epsilon}. \tag{15}$$

The trace is defined by,

$$Tr\left[G_l^{(trap)}(\lambda)\right] = \int_0^\infty r^2 dr G_l^{(trap)}(r,r;\lambda). \tag{16}$$

At infinite volume limit, the difference between trace of Green's functions of interacting and noninteracting systems is related to scattering phase shift through a dispersion integral, see, e.g., Refs. [51,54,65],

$$Tr\left[G_l^{(\infty)}(\epsilon) - G_l^{(0,\infty)}(\epsilon)\right] = -\frac{1}{\pi}\int_0^\infty d\lambda\frac{\delta_l^{(S)}(\lambda)}{(\lambda-\epsilon)^2}. \tag{17}$$

This relation is the result of Friedel formula [66] and Krein's theorem [67,68]. Equations (14) and (17) together lead to the same relation in Eq. (2), also see discussions in Refs. [51,53].

III. INTEGRATED CORRELATION FUNCTION FORMALISM WITH COULOMB INTERACTION

When the long-range Coulomb interaction is involved, the original relation in Eq. (2) cannot be applied directly, mainly due to the distortion in the asymptotic wavefunction, see, e.g., Ref. [69]. In this section, we explain what issues may arise from the inclusion of Coulomb interaction and how we can overcome the issues and modify Eq. (2).

The total interaction potential has two contributions,

$$V(r) = V_S(r) + V_C(r), \tag{18}$$

where $V_S(r)$ stands for a short-range potential, and $V_C(r)$ a long-range Coulomb potential between two electric charges Z_1 and Z_2,

$$V_C(r) = -\frac{Z}{r}, \quad \text{with} \quad Z = -Z_1 Z_2 e^2, \tag{19}$$

whose strength is represented by Z. The asymptotic behavior of infinite volume wavefunction is now given by, see, e.g., Ref. [32],

$$\psi_l^{(\infty)}(r;\epsilon) \xrightarrow{r\to\infty} \frac{4\pi i^l}{kr}\sin\left(kr - \frac{\pi l}{2} + \delta_l(\epsilon) - \gamma\ln(2kr)\right), \tag{20}$$

where $\gamma = -\frac{Z\mu}{k}$. The total partial phase shift,

$$\delta_l(\epsilon) = \delta_l^{(S)}(\epsilon) + \delta_l^{(C)}(\epsilon), \tag{21}$$

is the sum of short-range and long-range phase shifts. The Coulomb phase shift has the analytic expression in terms of gamma function Γ, see, e.g., Ref. [32],

$$\delta_l^{(C)}(\epsilon) = \arg\Gamma(l+1+i\gamma). \tag{22}$$

Using the distorted infinite volume asymptotic wavefunction in Eq. (20), and the identity relation in Eq. (8), we find

$$\int_0^\Lambda dr\left|u_l^{(\infty)}(r;k)\right|^2 \xrightarrow{\Lambda\to\infty} \frac{\Lambda - \frac{d}{dk}(\gamma\ln(2k\Lambda))}{2} + \frac{\sin(2k\Lambda - \pi l - 2\gamma\ln(2k\Lambda))}{4k} + \frac{1}{2}\frac{d\delta_l(\epsilon)}{dk}. \tag{23}$$

Clearly Eq. (23) has a different divergent asymptotic behavior from Eq. (11). Their difference is cutoff Λ dependent and diverges as $\Lambda\to\infty$. This is the primary reason that Eq. (2) cannot be applied directly when long-range Coulomb interaction is involved.

Fortunately, the asymptotic wavefunction with Coulomb interaction potential alone [32,69],

$$\psi_l^{(C,\infty)}(r;\epsilon) \xrightarrow{r\to\infty} \frac{4\pi i^l}{kr}\sin\left(kr - \frac{\pi l}{2} + \delta_l^{(C)}(\epsilon) - \gamma\ln(2kr)\right), \tag{24}$$

has the exact same form as Eq. (20) except with $\delta_l(\epsilon)$ replaced by $\delta_l^{(C)}(\epsilon)$. As a result, with only Coulomb interaction, we find

$$\int_0^\Lambda dr\left|u_l^{(C,\infty)}(r;k)\right|^2 \xrightarrow{\Lambda\to\infty} \frac{\Lambda - \frac{d}{dk}(\gamma\ln(2k\Lambda))}{2} + \frac{\sin(2k\Lambda - \pi l - 2\gamma\ln(2k\Lambda))}{4k} + \frac{1}{2}\frac{d\delta_l^{(C)}(\epsilon)}{dk}. \tag{25}$$

Therefore, the difference between Eqs. (23) and (25) yields the finite result,

$$\int_0^\Lambda dr\left[\left|u_l^{(\infty)}(r;k)\right|^2 - \left|u_l^{(C,\infty)}(r;k)\right|^2\right] \xrightarrow{\Lambda\to\infty} \frac{1}{2}\frac{d\delta_l^{(S)}(\epsilon)}{dk}. \tag{26}$$

Using the same steps as in Eqs. (12) and (13) and integration by parts, we arrive at the final expression in *Minkowski spacetime*,

$$C_l(t) - C_l^{(C)}(t) \xrightarrow{\text{trap}\to\infty} (2l+1)\frac{it}{\pi}\int_0^\infty d\epsilon\,\delta_l^{(S)}(\epsilon)e^{-i\epsilon t}. \tag{27}$$

Its counterpart in *Euclidean spacetime* can be obtained by an analytic continuation $t\to -i\tau$,

$$C_l(\tau) - C_l^{(C)}(\tau) \xrightarrow{\text{trap}\to\infty} (2l+1)\frac{\tau}{\pi}\int_0^\infty d\epsilon\,\delta_l^{(S)}(\epsilon)e^{-\epsilon\tau}. \tag{28}$$

Equation (27) bears a close resemblance to Eq. (2) in the absence of Coulomb interaction, except that the left-hand side now takes on new meanings. The $C_l(t)$ is the integrated correlation function for trapped particles interacting with both short-range potential and long-range Coulomb interaction, $C_l^{(C)}(t)$ with only Coulomb interaction instead of noninteracting $C_l^{(0)}(t)$, while $\delta_l^{(S)}(\epsilon)$ is the infinite volume phase shift from the short-range interaction only. Once $\delta_l^{(S)}$ is extracted from Eq. (27), the total phase

shift is simply given by adding to it the Coulomb phase shift in Eq. (22).

IV. NUMERICAL VERIFICATION WITH AN EXACTLY SOLVABLE MODEL

Having derived the Coulomb-modified relation in Eq. (27) or Eq. (28), it is important to check its validity. To this end, we employ an exactly solvable model in which every aspect of the problem is known in closed form.

For the short-range interaction, we adopt a contact interaction potential,

$$V_S(\mathbf{r}) = V_0 \frac{\delta(r)}{r^2}, \tag{29}$$

where V_0 is the bare potential strength. With a contact interaction, only S-wave ($l = 0$) phase shift will contribute, and its analytical solution in 3D is outlined in Appendix A. The phase shift is given by,

$$\delta_0^{(S)}(\epsilon) = \cot^{-1}\left(-\frac{1}{2\mu k V_R}\right) \xrightarrow{V_R \to 0} 0, \tag{30}$$

where V_R denotes renormalized contact interaction potential strength in Eq. (A8). The integration on the right-hand side of Eq. (27) can be carried out,

$$\frac{it}{\pi}\int_0^\infty d\epsilon \delta_0^{(S)}(\epsilon) e^{-i\epsilon t} = -\frac{1}{2}\mathrm{erfc}\left(\frac{1}{2\mu V_R}\sqrt{\frac{it}{2\mu}}\right) e^{\frac{1}{(2\mu V_R)^2}\frac{it}{2\mu}}, \tag{31}$$

in terms of complementary error function $\mathrm{erfc}(z) = 1 - \mathrm{erf}(z)$.

For the left-hand side of Eq. (27), we need to specify the trap and boundary conditions for the system, which will lead to quantized energies. The difference of integrated correlation functions can be computed from two energy spectra by,

$$C_l(t) - C_l^{(C)}(t) = \sum_n \left[e^{-i\epsilon_n t} - e^{-i\epsilon_n^{(C)} t}\right]. \tag{32}$$

The discrete energy levels ϵ_n and $\epsilon_n^{(C)}$ are the eigen-energies of Schrödinger equation in Eq. (5) for a trapped system with short-range plus Coulomb potential and pure Coulomb potential, respectively. Alternatively, the discrete energy levels can be obtained from Coulomb-modified Lüscher [1] or BERW [2] formulalike quantization conditions that connect short-range potential phase shifts with energy levels in the presence of Coulomb force,

$$\det\left[\delta_{lm_l,l'm_l'} \cot\delta_l^{(S)}(\epsilon) - \mathcal{M}^{(C)}_{lm_l,l'm_l'}(\epsilon)\right] = 0. \tag{33}$$

The definition of generalized zeta function in the presence of Coulomb force, $\mathcal{M}^{(C)}_{lm_l,l'm_l'}(\epsilon)$, can be found in Eq. (59) in Ref. [32]. In general, for commonly used traps, such as periodic finite box and harmonic oscillator traps, $\mathcal{M}^{(C)}_{lm_l,l'm_l'}(\epsilon)$ has to be solved numerically, which is a highly nontrivial task, see detailed discussion in Ref. [32].

For our purposes, we consider a simple trap: spherical hard-wall with radius R,

$$U_{trap}(r) = \begin{cases} 0, & r < R; \\ \infty, & \text{otherwise.} \end{cases} \tag{34}$$

In this trap, the quantization condition Eq. (33) is reduced to a simple form,

$$\cot\delta_l^{(S)}(\epsilon) = \frac{n_l^{(C)}(\gamma, kR)}{j_l^{(C)}(\gamma, kR)}. \tag{35}$$

The derivation is detailed in Appendix B, including the Coulomb-modified spherical Bessel functions $j_l^{(C)}(\gamma, kr)$ and $n_l^{(C)}(\gamma, kr)$ in Eqs. (B4) and (B5).

So the demonstration boils down to verifying the following relation,

$$C_0(\tau) - C_0^{(C)}(\tau) = \sum_n \left[e^{-\epsilon_n \tau} - e^{-\epsilon_n^{(C)}\tau}\right] \xrightarrow{R\to\infty} -\frac{1}{2}\mathrm{erfc}\left(\frac{1}{2\mu V_R}\sqrt{\frac{\tau}{2\mu}}\right) e^{\frac{1}{(2\mu V_R)^2}\frac{\tau}{2\mu}}. \tag{36}$$

We choose to work in Euclidean spacetime because of better convergence from exponential falloffs as opposed to oscillatory behavior in Minkowski spacetime. The ϵ_n are solved by Eq. (35) with $l = 0$, or equivalently

$$\delta_0^{(S)}(\epsilon_n) + \phi_0(\epsilon_n) = n\pi, \qquad n \in [0, 1, \ldots, \infty], \tag{37}$$

where we introduce a "trapped phase angle" ϕ_0 to rival the phase shift $\delta_0^{(S)}$ in infinite volume for notational convenience,

$$\phi_0(\epsilon) \equiv \cot^{-1}\left(-\frac{n_0^{(C)}(\gamma, kR)}{j_0^{(C)}(\gamma, kR)}\right) \xrightarrow{\gamma\to 0} \cot^{-1}\left(-\frac{n_0(kR)}{j_0(kR)}\right). \tag{38}$$

The $\epsilon_n^{(C)}$ with pure Coulomb interaction is solved by the quantization condition,

$$\phi_0(\epsilon_n^{(C)}) = n\pi, \qquad n \in [0, 1, \ldots, \infty]. \tag{39}$$

The pole position of $\cot\phi_0$ must be computed numerically by using Eq. (39), however at the limit of $\gamma \to 0$ (a pure

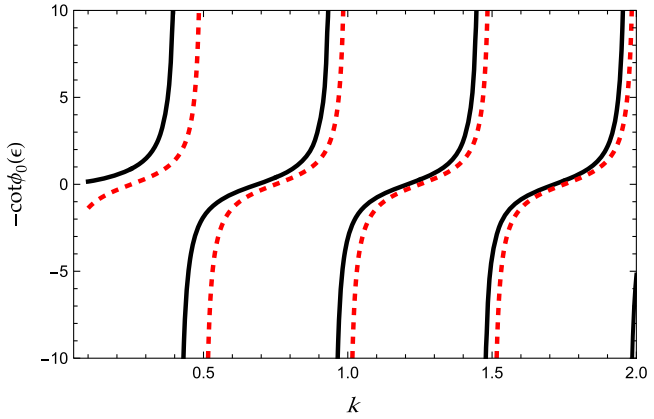


FIG. 1. Coulomb effects in the generalized zeta function in Eq. (38): the Coulomb-corrected $(-\cot\phi_0)$ (solid black) vs its non-Coulomb limit (dashed red) at trap radius $R = 2\pi$. The reduced mass is taken as $\mu = 1$ and Coulomb potential strength as $Z = 0.1$. The pole position at non-Coulomb limit is simply given by $k_n = \frac{n\pi}{R} = \frac{n}{2}$, where $n \in [0, 1, \ldots]$. With Coulomb correction, pole positions are shifted by Coulomb potential, and must be numerically solved by Eq. (39).

spherical hard wall trap), the pole positions are simply given by $\epsilon_n = \frac{1}{2\mu}(\frac{n\pi}{R})^2$, where $n \in [0, 1, \ldots]$.

The effects of Coulomb interaction in the generalized zeta function are demonstrated in Fig. 1. We see that Coulomb corrections can be fairly significant at low energies, and become smaller as energy is increased.

In Fig. 2, we show how the quantization condition in Eq. (37), or equivalently Eq. (35), works. The $\cot\delta_0^{(S)}$ from the infinite volume phase shift in Eq. (30) is plotted as a function of center of mass momentum k (red curve). On the

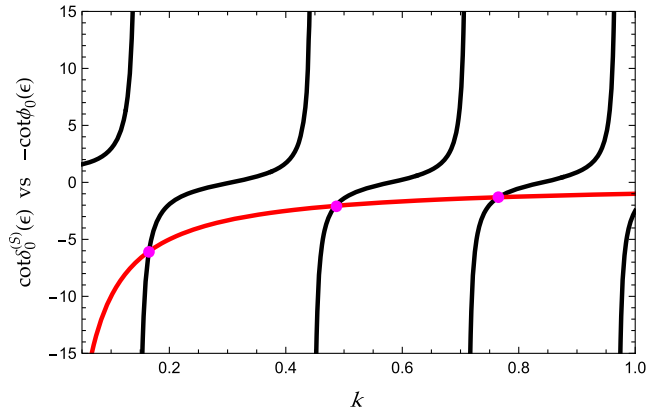


FIG. 2. Quantization condition plot of Eq. (37) for two particles interacting through a contact potential of strength V_0 and Coulomb potential of strength Z in a spherical hard-wall trap of radius R. The black curves correspond to the Coulomb-corrected "trapped phase angle" (ϕ_0) and the red curve to the infinite volume phase shift $(\delta_0^{(S)})$. The quantized energy levels are at the intersection points (purple dots) of black and red curves. The parameters are taken as: $V_R = 0.5$, $Z = 0.1$, $R = 4\pi$, $\mu = 1$.

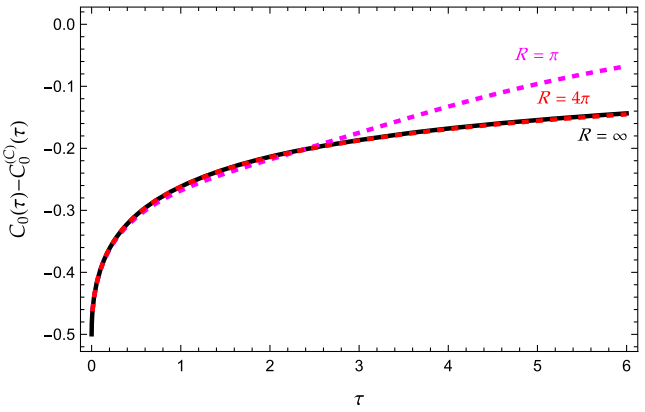


FIG. 3. Convergence of Eq. (36). The difference of integrated correlation functions (dashed red) at two values of trap radius $R = \pi$ (dashed purple), 4π (dashed red) vs the result of a weighted integral from infinite volume phase shifts (solid black). The rest of the parameters are taken as: $V_R = 0.5$, $\mu = 1$, and $Z = 0.1$.

same graph the generalized zeta function $(-\cot\phi_0)$ from Eq. (38) is also plotted (black curves), where the two intercept gives rise to quantized energy levels in the system. Each quantized energy level is found between two neighboring poles of the generalized zeta function, which correspond to the noninteracting levels in the trap. This is to be expected because interaction only causes the noninteracting levels to shift. The amount of energy shift is characterized by the infinite volume phase shifts.

Finally, we show in Fig. 3 how the Coulomb-modified formula in Eq. (36) is satisfied. The right-hand side from the infinite volume phase shift is plotted as a function of Euclidean time τ (black curve). The left-hand side is obtained from summing over two energy spectra ϵ_n and $\epsilon_n^{(C)}$. The formula requires the limit of infinite trap size. So we evaluate it at two values of the hard-wall radius R (colored curves). About a hundred energy levels are required to saturate the sum. We see a rapid convergence of the relation over a wide range of times as the trap size is increased. Moreover, the convergence is faster at earlier times.

V. SUMMARY AND OUTLOOK

The integrated correlation function formalism developed for scattering in Refs. [51–53] is now extended to include long-range Coulomb interaction for charged particle systems. The central result is the Coulomb-modified relation in Eq. (27) or its Euclidean counterpart in Eq. (28). Remarkably, it retains the same form as the original Eq. (2) in the absence of Coulomb interaction, but with a new meaning. On the left-hand side, instead of the difference between interacting and noninteracting integrated correlation functions for a short-range potential, it is the difference between short-range plus Coulomb potential and

pure Coulomb potential. On the right-hand side, it involves the infinite volume phase shift due to short-range potential only. The realization comes from a careful examination of the asymptotic behavior of the formalism in the presence of Coulomb interaction. The new relation is free of cutoff dependence and divergences, with a well-defined approach to the infinite volume limit. The relation is verified to high precision with an exactly solvable model: a contact interaction potential and a spherical hard-wall trap. Several additional comments are in order.

The relation is given in $3+1$ dimensions in a partial-wave projection. It is valid for any short-range interaction that can be described by a central potential. The trap used to contain the system can either have continuous rotational symmetry (hard-wall, harmonic oscillator, etc.) or discrete symmetry (periodic boxes/lattices) in which case a projection to the irreducible representations of the symmetry group is required.

It is worth emphasizing two properties of the integrated correlation function formalism, in comparison to Lüscher-like quantization conditions: (a) it only requires correlation functions, not energy spectrum (even though an energy spectral representation can be used as in our numerical verification); and (b) it has faster convergence at smaller Euclidean times. Both properties bode well for lattice QCD simulations of multibaryon systems where signal-to-noise ratio and energy spectrum extraction present major challenges, especially when large volumes are involved.

In practical applications, the extraction of phase shift from the integrated correlation function formalism is essentially an *inverse problem* for which there are well-established methods in the literature, see, e.g., Refs. [70–72].

Although the derivation is based on nonrelativistic dynamics, we envision no conceptual issues extending it to relativistic dynamics [52].

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DATA AVAILABILITY

No data were created or analyzed in this study.

APPENDIX A: SCATTERING SOLUTIONS WITH A CONTACT INTERACTION IN INFINITE VOLUME

In infinite volume, with a incoming plane wave of $e^{i\mathbf{k}\cdot\mathbf{r}}$, the scattering solution of two particle interaction is described by the inhomogeneous integral Lippmann-Schwinger (LS) equation,

$$\psi_\epsilon^{(\infty)}(\mathbf{r},\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \int_{-\infty}^{\infty} d\mathbf{r}' G^{(0,\infty)}(\mathbf{r}-\mathbf{r}';\epsilon) \times V_S(\mathbf{r}')\psi_\epsilon^{(\infty)}(\mathbf{r}',\mathbf{k}), \tag{A1}$$

where $k=\sqrt{2\mu\epsilon}$, and the noninteracting Green's function is given by

$$G^{(0,\infty)}(\mathbf{r};\epsilon) = \int \frac{d\mathbf{p}}{(2\pi)^3}\frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{\frac{q^2}{2\mu}-\frac{\mathbf{p}^2}{2\mu}} = -\frac{2\mu}{4\pi} ikh_0^{(+)}(k|\mathbf{r}|). \tag{A2}$$

With a contact interaction $V_S(\mathbf{r}) = V_0\frac{\delta(r)}{r^2}$, the LS equation is reduced to

$$\psi_\epsilon^{(\infty)}(\mathbf{r},\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{r}} - i2\mu k V_0 h_0^{(+)}(kr)\psi_\epsilon^{(\infty)}(0,\mathbf{k}). \tag{A3}$$

Hence only the S wave contributes to scattering solutions,

$$\psi_0^{(\infty)}(r;\epsilon) = 4\pi j_0(kr) - i2\mu k V_0 h_0^{(+)}(kr)\psi_0^{(\infty)}(0;\epsilon), \tag{A4}$$

where the partial wave expansion is defined by

$$\psi_\epsilon^{(\infty)}(\mathbf{r},\mathbf{k}) = \sum_{lm_l} Y_{lm_l}^*(\hat{\mathbf{k}})\psi_l^{(\infty)}(r;\epsilon)Y_{lm_l}(\hat{\mathbf{r}}). \tag{A5}$$

The formal solution is thus given by

$$\psi_0^{(\infty)}(r;\epsilon) = 4\pi j_0(kr) + 4\pi i t_0^{(S)}(\epsilon)h_0^{(+)}(kr), \tag{A6}$$

where the scattering amplitude is defined by

$$t_0^{(S)}(\epsilon) = -\frac{2\mu k}{\frac{1}{V_0} + i2\mu k h_0^{(+)}(kr)|_{r\to 0}}. \tag{A7}$$

Using asymptotic behavior of spherical Hankel function: $h_0^{(+)}(kr)|_{r\to 0} \to 1-\frac{i}{kr}$, and also introducing the renormalized coupling strength by

$$V_R = \left(\frac{1}{V_0} + \frac{2\mu}{r}\bigg|_{r\to 0}\right)^{-1}, \tag{A8}$$

the scattering amplitude now is given by

$$t_0^{(S)}(\epsilon) = -\frac{1}{\frac{1}{2\mu V_R k} + i}. \tag{A9}$$

The scattering phase shift due to contact interaction is hence given by

$$\cot\delta_0^{(S)}(\epsilon) = i + \frac{1}{t_0^{(S)}(\epsilon)} = -\frac{1}{2\mu V_R k}. \tag{A10}$$

APPENDIX B: CONNECTING EIGENSOLUTIONS IN A TRAP TO INFINITE VOLUME SCATTERING SOLUTIONS WITH COULOMB INTERACTION

In this appendix, we discuss some exact solutions involving Coulomb interaction. They are needed in the validation of the new relation in Eq. (27).

1. Exact solution of partial-wave-projected Green's function for pure Coulomb interaction

In addition to the asymptotic wavefunction in Eq. (20) and the phase shift in Eq. (22), the Green's function also has an analytical expression for Coulomb interaction. The Green's function for l-th partial wave is the solution of the differential equation,

$$\left[\epsilon+\frac{1}{2\mu r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)-\frac{l(l+1)}{2\mu r^2}-V_C(r)\right]G_l^{(C,\infty)}(r,r';\epsilon)=\frac{\delta(r-r')}{r^2}, \tag{B1}$$

whose analytical expression is given by [32,69,73],

$$G_l^{(C,\infty)}(r,r';\epsilon)=-i2\mu k j_l^{(C)}(\gamma,kr_<)h_l^{(C,+)}(\gamma,kr_>), \tag{B2}$$

where $r_<$ and $r_>$ represent the lesser and greater of (r,r'), respectively, and

$$h_l^{(C,\pm)}(\gamma,kr)=j_l^{(C)}(\gamma,kr)\pm in_l^{(C)}(\gamma,kr). \tag{B3}$$

The Coulomb-modified spherical Bessel functions $j_l^{(C)}(\gamma,kr)$ and $n_l^{(C)}(\gamma,kr)$ are defined [32] via two linearly independent Kummer functions $M(a,b,z)$ and $U(a,b,z)$,

$$j_l^{(C)}(\gamma,kr)=\mathbb{C}_l(\gamma)(kr)^l e^{ikr}M(l+1+i\gamma,2l+2,-2ikr), \tag{B4}$$

and

$$\begin{aligned}n_l^{(C)}(\gamma,kr)&=i(-2kr)^l e^{\frac{\pi}{2}\gamma}e^{ikr}U(l+1+i\gamma,2l+2,-2ikr)e^{i\delta_l^{(C)}}\\&\quad-i(-2kr)^l e^{\frac{\pi}{2}\gamma}e^{-ikr}U(l+1-i\gamma,2l+2,2ikr)e^{-i\delta_l^{(C)}}.\end{aligned} \tag{B5}$$

The Sommerfeld factor is defined by [69],

$$\mathbb{C}_l(\gamma)=2^l\frac{|\Gamma(l+1+i\gamma)|}{(2l+1)!}e^{-\frac{\pi}{2}\gamma}. \tag{B6}$$

The Coulomb phase shift, $\delta_l^{(C)}$, is defined in Eq. (22).

2. Coulomb-modified scattering solutions with a contact interaction in infinite volume

In infinite volume (no trap), the scattering solution of two charged particles interacting via a Coulomb potential is described by the inhomogeneous LS equation, see, e.g., Ref. [32],

$$\psi_\epsilon^{(\infty)}(\mathbf{r},\mathbf{k})=\psi_\epsilon^{(C,\infty)}(\mathbf{r},\mathbf{k})+\int_{-\infty}^{\infty}d\mathbf{r}'G^{(C,\infty)}(\mathbf{r},\mathbf{r}';\epsilon)\times V_S(\mathbf{r}')\psi_\epsilon^{(\infty)}(\mathbf{r}',\mathbf{k}), \tag{B7}$$

where $\psi_\epsilon^{(C,\infty)}(\mathbf{r},\mathbf{k})$ is Coulomb wavefunction and $G^{(C,\infty)}(\mathbf{r},\mathbf{r}';\epsilon)$ is Coulomb Green's function.

In the case of a contact interaction $V_S(\mathbf{r})=V_0\frac{\delta(r)}{r^2}$, only S-wave will contribute, so after partial-wave projection, we find

$$\psi_0^{(\infty)}(r;\epsilon)=\psi_0^{(C,\infty)}(r;\epsilon)+V_0G_0^{(C,\infty)}(r,0;\epsilon)\psi_0^{(\infty)}(0;\epsilon), \tag{B8}$$

where the analytic expression of S-wave Coulomb wave function and Coulomb Green's function are given by

$$\psi_0^{(C,\infty)}(r;\epsilon)=4\pi j_0^{(C)}(\gamma,kr)e^{i\delta_0^{(C)}(\epsilon)}, \tag{B9}$$

and

$$G_0^{(C,\infty)}(r,r';\epsilon)=-i2\mu k j_0^{(C)}(\gamma,kr_<)h_0^{(C,+)}(\gamma,kr_>). \tag{B10}$$

The formal scattering solution in the presence of Coulomb force can thus be obtained,

$$\psi_0^{(\infty)}(r;\epsilon)=4\pi j_0^{(C)}(\gamma,kr)e^{i\delta_0^{(C)}(\epsilon)}+4\pi i t_0^{(SC)}(\epsilon)h_0^{(C,+)}(\gamma,kr)e^{-i\delta_0^{(C)}(\epsilon)}, \tag{B11}$$

where

$$t_0^{(SC)}(\epsilon)=\frac{-2\mu k\mathbb{C}_0^2(\gamma)e^{2i\delta_0^{(C)}(\epsilon)}}{\frac{1}{V_0}-\mathrm{Re}\left[G_0^{(C,\infty)}(r,0;\epsilon)|_{r\to0}\right]+i2\mu k\mathbb{C}_0^2(\gamma)}. \tag{B12}$$

The $t_0^{(SC)}(\epsilon)$ is usually parametrized by

$$t_0^{(SC)}(\epsilon)=\frac{1}{\cot\delta_0^{(S)}(\epsilon)-i}e^{2i\delta_0^{(C)}(\epsilon)}. \tag{B13}$$

Hence we find a useful relation

$$\frac{1}{V_0} = -2\mu k \mathbb{C}_0^2(\gamma)\cot\delta_0^{(S)}(\epsilon) + \mathrm{Re}\left[G_0^{(C,\infty)}(r,0;\epsilon)|_{r\to 0}\right]. \tag{B14}$$

The total scattering amplitude is defined by

$$t_0(\epsilon) = t_0^{(C)}(\epsilon) + t_0^{(SC)}(\epsilon) = \frac{e^{2i\delta_0(\epsilon)}-1}{2i}, \tag{B15}$$

where $t_0^{(C)}(\epsilon)$ is pure Coulomb scattering amplitude

$$t_0^{(C)}(\epsilon) = \frac{e^{2i\delta_0^{(C)}(\epsilon)}-1}{2i} = \frac{1}{\cot\delta_0^{(C)}(\epsilon) - i}, \tag{B16}$$

and $\delta_0(\epsilon)$ is total S-wave scattering amplitude,

$$\delta_0(\epsilon) = \delta_0^{(S)}(\epsilon) + \delta_0^{(C)}(\epsilon). \tag{B17}$$

With Coulomb correction, the Friedel formula and Krein's theorem in Eq. (17) must be replaced by,

$$Tr\left[G_l^{(\infty)}(\epsilon) - G_l^{(C,\infty)}(\epsilon)\right] = -\frac{1}{\pi}\int_0^\infty d\lambda \frac{\delta_l^{(S)}(\lambda)}{(\lambda-\epsilon)^2}, \tag{B18}$$

where $G_l^{(\infty)}(\epsilon)$ and $G_l^{(C,\infty)}(\epsilon)$ represent Green's function operators with short-range plus Coulomb interaction and only Coulomb interaction, respectively. The infinite volume Green's function, $G_l^{(\infty)}(r,r';\epsilon)$, satisfies the Dyson equation,

$$\begin{aligned} G_l^{(\infty)}(r,r';\epsilon) &= G_l^{(C,\infty)}(r,r';\epsilon) \\ &+ \int_0^\infty r''^2 dr'' G_l^{(C,\infty)}(r,r'';\epsilon) \\ &\times V_S(r'') G_l^{(\infty)}(r'',r';\epsilon). \end{aligned} \tag{B19}$$

3. Coulomb-modified quantization condition in spherical hard-wall trap with a contact interaction

The dynamics of a particles system in a trap can be also described by the homogeneous Lippmann-Schwinger equation,

$$\psi(\mathbf{r};\epsilon) = \int d\mathbf{r}' G^{(C,trap)}(\mathbf{r},\mathbf{r}';\epsilon) V_S(\mathbf{r}')\psi(\mathbf{r}';\epsilon), \tag{B20}$$

where $G^{(C,trap)}(\mathbf{r},\mathbf{r}';\epsilon)$ is the Coulomb-modified Green's function for the trapped system, and it satisfies the differential equation,

$$\left[\epsilon + \frac{\nabla^2}{2\mu} - U_{trap}(r) - V_C(r)\right] G^{(C,trap)}(\mathbf{r},\mathbf{r}';\epsilon) = \delta(\mathbf{r}-\mathbf{r}'). \tag{B21}$$

The partial wave expansion of Green's function is defined by

$$G^{(C,trap)}(\mathbf{r},\mathbf{r}';\epsilon) = \sum_{lm_l} Y_{lm_l}(\hat{\mathbf{r}}) G_l^{(C,trap)}(r,r';\epsilon) Y_{lm_l}^*(\widehat{\mathbf{r}'}). \tag{B22}$$

For a spherical hard-wall trap, the analytical form of the Coulomb-modified partial wave Green's function for the trapped system can be obtained, see Eq. (73) in Ref. [32],

$$\begin{aligned} G_l^{(C,trap)}(r,r';\epsilon) &= -2\mu k j_l^{(C)}(\gamma,kr_<) j_l^{(C)}(\gamma,kr_>) \\ &\times \left[\frac{n_l^{(C)}(\gamma,kR)}{j_l^{(C)}(\gamma,kR)} - \frac{n_l^{(C)}(\gamma,kr_>)}{j_l^{(C)}(\gamma,kr_>)}\right], \end{aligned} \tag{B23}$$

where the Coulomb-modified $j_l^{(C)}(\gamma,kr)$ and $n_l^{(C)}(\gamma,kr)$ functions are defined in Eqs. (B4) and (B5), respectively.

With a contact interaction $V_S(\mathbf{r}) = V_0\frac{\delta(r)}{r^2}$, after the S-wave projection, Eq. (B20) yields a quantization condition,

$$\frac{1}{V_0} = G_0^{(C,trap)}(r,0;\epsilon)|_{r\to 0}. \tag{B24}$$

Using the relation in Eq. (B14), we find

$$\cot\delta_0^{(S)}(\epsilon) = \frac{Re[G_0^{(C,\infty)}(r,0;\epsilon)|_{r\to 0}] - G_0^{(C,trap)}(r,0;\epsilon)|_{r\to 0}}{2\mu k \mathbb{C}_0^2(\gamma)}. \tag{B25}$$

The real part of the Coulomb Green's function in infinite volume is given by

$$Re\left[G_0^{(C,\infty)}(r,r';\epsilon)\right] = 2\mu k j_0^{(C)}(\gamma,kr_<) n_0^{(C)}(\gamma,kr_>), \tag{B26}$$

which cancels out the second term of the Coulomb Green's function in the trap in Eq. (B23). Also using the asymptotic form

$$j_0^{(C)}(\gamma,kr) \xrightarrow{r\to 0} \mathbb{C}_0(\gamma), \tag{B27}$$

the Coulomb-modified quantization condition for a contact interaction potential is found in Eq. (35).

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