Toward extracting the scattering phase shift from integrated correlation functions

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In present work, a relation that connects the integrated correlation function of a trapped two-particle system to infinite volume particles scattering phase shift is derived. It has the potential to provide an alternative approach for extracting two-particle scattering phase shift from integrated correlation function in lattice simulation at small Euclidean time region. Both (i) perturbation calculation of $(1+1)$-dimensional lattice Euclidean field theory model of fermions interacting with a contact interaction and (ii) Monte Carlo simulation of a 1D exactly solvable quantum mechanics model are carried out to test the proposed relation. In contrast to conventional two-step approach of extracting energy levels from temporal correlation function in lattice simulation at large Euclidean time first and then applying Lüscher formula to convert energy levels into scattering phase shifts, we show that the difference of integrated correlation functions between interacting and noninteracting trapped systems converges rapidly to infinite volume limit that is given in terms of scattering phase shifts at small Euclidean time region.

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I. INTRODUCTION

Study of hadron/nuclear particles interactions and properties of few-body resonances from the first principles, quantum chromodynamics (QCD) that is the underlying theory of quark and gluon interactions, is one of the major tasks in modern hadron/nuclear physics. In particular hadron/nuclear particles provide the only means of understanding the quark and gluon dynamics. However, extracting information of hadron/nuclear particle interactions from the first principles, such as scattering phase shifts, is not always straightforward. Usually theoretical computations are performed in various traps, for instance, periodic cubic box in lattice quantum chromodynamics (LQCD) and harmonic oscillator trap in nuclear physics. As the result of trapped systems, the energy spectra become discrete. To extract the scattering information, normally the two-step procedures are carried out: (1) First of all, discrete low-lying few-body energy levels are extracted by fitting exponential decaying behavior of correlation functions in Euclidean space-time, and looking for the plateau in temporal correlation functions when Euclidean time is large enough so that all excited energy levels decay off rapidly and only lowest energy level becomes dominant. The energy spectra of excited states can be extracted in a similar way by applying variational approach and generalized eigenvalue method [1–3]; (2) Applying the Lüscher formula [4] in LCQD or Busch-Englert-Rzażewski-Wilkens (BERW) formula [5] in a harmonic oscillator (h.o.) trap in nuclear physics, the discrete energy spectra of trapped system can be converted into scattering phase shifts, etc. The Lüscher formula and BERW formula have been quickly extended to include inelastic effects, such as coupled-channel effect and three-body problems, etc.; see, e.g., Refs. [6–45]. This two-step approach has been proven very successful in number of applications especially in meson sector; see, e.g., Refs. [29,46–57]. However, the two-step approach also display some disadvantages that are summarized nicely in Ref. [58] such as the determination of energy levels in large spatial volume becomes difficult, etc. The situation is even more challenging in the baryon sector, finding a clear signal of a stable plateau in nucleon-nucleon reaction correlation functions and pulling out energy spectra from the noisy lattice simulation data is already a difficult task. Therefore, there have been a number of proposals to explore alternative approaches in recent years, such as determining scattering amplitudes from finite-volume spectral functions in Ref. [58] and extraction of spectral densities from lattice correlators in Refs. [59,60], etc.

In this work, we will establish a connection between integrated correlation functions and scattering phase shift that has the potential to provide an alternative approach of

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extracting scattering phase shifts from lattice QCD calculation and show the following:

(i) The difference of integrated trapped two-particle correlation functions between interacting particles system and free particles system in $1+1$ space-time dimensions is related to infinite volume particles scattering phase shift, $\delta(\epsilon)$, by

$$C(t) - C_0(t) \underset{t=-i\tau}{\overset{\text{trap}\to\infty}{\to}} \frac{1}{\pi}\int_0^\infty d\epsilon \frac{d\delta(\epsilon)}{d\epsilon} e^{-\epsilon\tau} + \frac{\delta(0)}{\pi}, \quad (1)$$

where $C(t)$ and $C_0(t)$ are integrated correlation functions for two interacting and noninteracting particles in a trap, respectively, and τ stands for Euclidean time.

(ii) Integrated trapped correlation functions are given in terms of eigenenergies of two particles by

$$C(t) - C_0(t) \overset{t=-i\tau}{=} \sum_n [e^{-\epsilon_n \tau} - e^{-\epsilon_n^{(0)}\tau}], \quad (2)$$

where ϵ_n and $\epsilon_n^{(0)}$ are eigenenergies of two interacting and noninteracting particles in a trap, respectively. Hence integrated trapped correlation functions resemble the partition function in statistical mechanics,

$$C(t) - C_0(t) \overset{\tau\leftrightarrow\beta}{\leftrightarrow} \mathrm{Tr}[e^{-\beta\hat{H}} - e^{-\beta\hat{H}_0}], \quad (3)$$

with τ playing the role of $\beta = \frac{1}{k_B T}$. $\hat{H}$ and $\hat{H}_0$ are interacting and noninteracting particles Hamiltonian operators respectively. The relation given in Eq. (1) therefore is analogous to the well-known result in the calculation of the second virial coefficient of quantum gas by a virial expansion approach (also known as cluster expansion method) in quantum statistical mechanics, see, e.g., Refs. [61,62].

(iii) As discussed in Ref. [62], at high temperature, the scattering cross section is of the order the square of the thermal de Broglie wavelength, which becomes much smaller than the average interparticle distance in quantum gas systems, hence the inclusion of only few-body correlations in quantum virial expansion has proven already sufficient at high temperature (small β) in describing and understanding properties of quantum gas systems. In a similar situation, two distinct physical scales in integrated trapped correlation functions are (1) the Euclidean evolving time τ that plays the role of square of the thermal de Broglie wavelength and (2) the size of trap, L. When τ is much smaller than L, the difference of integrated trapped two-particle correlation functions can be described by series expansion in terms of powers of τ/L, we may expect that the difference of integrated trapped two-particle correlation functions rapidly approaches the infinite volume limit that is given in terms of scattering phase shifts in Eq. (1) at small τ region even with a modest size of trap. This conclusion as matter of fact can be easily illustrated by using relation listed in Eq. (3), near small $\tau \sim 0$, by Taylor expansion

$$e^{-\hat{H}\tau} \sim (1 - \hat{V}\tau + \cdots) e^{-\hat{H}_0\tau},$$

where $\hat{V} = \hat{H} - \hat{H}_0$ stands for interaction operator, we can show that

$$C(t) - C_0(t) \overset{\tau\sim 0}{\approx} -\langle \hat{V}(\tau)\rangle\tau + \mathcal{O}(\langle \hat{V}(\tau)\rangle^2\tau^2), \quad (4)$$

where $\langle \hat{V}(\tau)\rangle = \mathrm{Tr}[\hat{V}e^{-\hat{H}_0\tau}]$ may be interpreted as thermal average of particles interaction that is proportional to the inverse size of trap: $\langle \hat{V}(\tau)\rangle \propto \frac{1}{L}$. Therefore, as $\tau/L \ll 1$, a thermal de Broglie wavelength is much smaller than the size of a trap, particles becomes less aware of the finite size of a trap, and the difference of integrated trapped two-particle correlation functions agree well with the infinite volume limit result even with finite size of a trap. This observation is further illustrated analytically in great details by perturbation calculation of two-fermion correlation function of a simple lattice field theory model in Sec. IV.

(iv) Another one of our primary goals in this work is thus first to illustrate numerically that two sides in Eq. (1) indeed display a rather good agreement at small τ region even with a modest size of the trap, as the size of trap is increased, the agreement then starts expand into larger τ region, and second to establish the possibility of extracting the infinite volume particles scattering phase from Monte Carlo calculation of integrated correlation functions of trapped two-particle system at small τ region. The Monte Carlo simulation test of a quantum mechanical model with a spinless particle interacting with a square well potential in a harmonic trap is carried out in this work in Sec. V. Monte Carlo data indeed show a good agreement with infinite volume limit near small τ region, and the range of agreement in τ start expanding as the size of trap is increased.

We remark that, at the current scope, all our discussions are only limited to nonrelativistic dynamics in one spatial and one temporal dimensional space-time, and a lot of more studies must to be conducted to include relativistic dynamics and inelastic effect, etc. before it can be applied to realistic cases in lattice QCD calculation.

The paper is organized as follows. First of all, a field theory model for the study of nonrelativistic fermions interaction in a trap is set up in Sec. II, the dynamics of two fermions interaction in a trap and the two-particle correlation function are also presented in Sec. II. The derivation of the infinite volume limit of integrated two-particle correlation function, and its relation to particles scattering phase shift are given in Sec. III. The perturbation calculation of two fermions correlation function of a lattice field theory is carried out and presented in Sec. IV. The $1+1$D Monte Carlo simulation test with a exact solvable quantum mechanics model is presented and discussed in Sec. V. The discussions and summary are given in Sec. VI.

II. A FIELD THEORY MODEL FOR NONRELATIVISTIC FERMIONS INTERACTION IN A TRAP

In this section, we first setup a $(1+1)$-dimensional field theory model for the study of two nonrelativistic fermions interaction in a trap. All the conventions are established in Sec. II A, the dynamical equations of two particles interaction are presented in Sec. II B, and the definition of time forward propagating two-particle correlation function is given in Sec. II C.

A. A field theory model setup

To restrain our current discussion in the case of single species nonrelativistic particles interaction, a simple $(1+1)$- dimensional nonrelativistic field theory model of spin-$1/2$ fermions interaction via a short-range potential in a trap is adopted in this work. Hamiltonian operator of the trapped fermions system is

$$\hat{H} = \sum_{\sigma=\uparrow,\downarrow} \int dx \hat{\psi}^\dagger_\sigma(x) \left[-\frac{1}{2m}\frac{d^2}{dx^2} + U(x) \right] \hat{\psi}_\sigma(x) + \frac{1}{2}\int dxdy \hat{\psi}^\dagger_\uparrow(x)\hat{\psi}^\dagger_\downarrow(y) V(x-y) \hat{\psi}_\downarrow(y)\hat{\psi}_\uparrow(x), \quad (5)$$

where $\sigma = \uparrow, \downarrow$ and m refer to the fermion polarizations and mass, respectively, and $\hat{\psi}_\sigma(x)$ stands for the fermion field operator. The trap potential and short-range interaction potential between two fermions with opposite polarizations are represented by $U(x)$ and $V(x-y)$, respectively. Only spatially symmetric short-range interaction is considered in this work:

$$V(x-y) = V(y-x),$$

hence, the interaction between two fermions with the same polarizations is suppressed by Pauli exclusive principle.

The second quantization representation of Hamiltonian operator can be obtained by using the following relations:

$$\hat{\psi}_\sigma(x) = \sum_n \varphi_n(x) a_{n,\sigma}, \qquad \hat{\psi}^\dagger_\sigma(x) = \sum_n \varphi^*_n(x) a^\dagger_{n,\sigma}, \quad (6)$$

where $a_{n,\sigma}$ and $a^\dagger_{n,\sigma}$ are the annihilation and creation operators for a single fermion state that is labeled by quantum numbers of (n,σ). The expansion coefficient, $\varphi_n(x)$, is the eigen wave function of single particle state in the trap corresponding to the eigenenergy of $\epsilon^{(0)}_n$, and it satisfies a Hartree-Fock-like equation, see, e.g., Ref. [63],

$$\left[-\frac{1}{2m}\frac{d^2}{dx^2} + U(x) \right] \varphi_n(x) = \epsilon^{(0)}_n \varphi_n(x). \quad (7)$$

The second quantization representation of Hamiltonian of trapped fermions system is thus given by

$$\hat{H} = \sum_{\sigma,n} \epsilon^{(0)}_n a^\dagger_{\sigma,n} a_{\sigma,n} + \frac{1}{2} \sum_{n_1,n_2,n'_1,n'_2} V_{n'_1,n'_2;n_1,n_2} a^\dagger_{\uparrow,n_1} a^\dagger_{\downarrow,n_2} a_{\downarrow,n'_2} a_{\uparrow,n'_1}, \quad (8)$$

where

$$V_{n'_1,n'_2;n_1,n_2} = \int dxdy \varphi^*_{n'_1}(x)\varphi^*_{n'_2}(y) V(x-y) \varphi_{n_1}(x)\varphi_{n_2}(y). \quad (9)$$

B. Two fermions interaction in a trap

The two-particle state is defined in this subsection and dynamical equation of trapped two interacting fermions system is also presented. We remark that the subscript of spatial integration of a trapped system, $\int_{\text{trap}} dx$, is suppressed in follows: the spatial integration of a trapped system for a periodic box and harmonic oscillator trap is understood as

$$\int dx = \begin{cases} \int_0^L dx, & \text{for a periodic box of size } L \\ \int_{-\infty}^{\infty} dx, & \text{for a h.o. trap} \end{cases}. \quad (10)$$

1. Spin singlet state of two fermions in a trap

The state of two fermions with a total spin-S and interacting with a short-range potential in a trap is defined by

$$|E\rangle = \sum_{\sigma_1,\sigma_2} \int dx_1 dx_2 \Psi_E(x_1,x_2) \chi^{(S)}_{\sigma_1,\sigma_2} \frac{\hat{\psi}^\dagger_{\sigma_1}(x_1)\hat{\psi}^\dagger_{\sigma_2}(x_2)}{\sqrt{2}} |0\rangle, \quad (11)$$

where $\Psi_E(x_1,x_2)$ and $\chi^{(S)}_{\sigma_1,\sigma_2}$ are spatial and spin wave functions of two fermions system with total spin-S, respectively. The factor $1/\sqrt{2}$ takes into account the exchange symmetry of two distinguishable fermions. For spatially symmetric short-range interaction potentials, such as a contact interaction, the antisymmetric spatial wave function is highly suppressed. Hence only spin single state with total spin-($S=0$) is considered in the current work,

$$\chi^{(S=0)}_{\sigma_1,\sigma_2} = \frac{1}{\sqrt{2}}(\delta_{\sigma_1,\uparrow}\delta_{\sigma_2,\downarrow} - \delta_{\sigma_1,\downarrow}\delta_{\sigma_2,\uparrow}), \tag{12}$$

and spatial wave function is symmetric under exchange of coordinates of two particles,

$$\Psi_E(x_1,x_2) = \Psi_E(x_2,x_1). \tag{13}$$

The second quantization representation of two-fermion state is given by

$$|E\rangle = \frac{1}{2}\sum_{n_1,n_2}\tilde{\Psi}_E(n_1,n_2)(a^\dagger_{\uparrow,n_1}a^\dagger_{\downarrow,n_2} - a^\dagger_{\downarrow,n_1}a^\dagger_{\uparrow,n_2})|0\rangle, \tag{14}$$

where

$$\tilde{\Psi}_E(n_1,n_2) = \int dx_1 dx_2 \Psi_E(x_1,x_2)\varphi^*_{n_1}(x_1)\varphi^*_{n_2}(x_2), \tag{15}$$

and it is symmetric under exchange of two-particle state indices,

$$\tilde{\Psi}_E(n_1,n_2) = \tilde{\Psi}_E(n_2,n_1). \tag{16}$$

In the basis of single particle wave functions, the two-fermion spatial wave function is thus given by

$$\Psi_E(x_1,x_2) = \sum_{n_1,n_2}\tilde{\Psi}_E(n_1,n_2)\varphi_{n_1}(x_1)\varphi_{n_2}(x_2). \tag{17}$$

The orthogonality of two-fermion states,

$$\langle E|E'\rangle = \delta_{E,E'}$$

yields that the spatial wave functions are orthonormal and

$$\sum_{n_1,n_2}\tilde{\Psi}^*_{E'}(n_1,n_2)\tilde{\Psi}_E(n_1,n_2) = \delta_{E,E'}. \tag{18}$$

We remark that our current discussion is restricted to only a two-particle elastic region, so that the Fock space expansion in Eqs. (11) and (14) is only limited to a two-particle state contribution, the multiparticle states with a number of particles equal or greater than 3 are all neglected for now.

2. Dynamical equation of trapped two-fermion system

The effective dynamical equation for two-particle state can be derived from the variational principle by evaluating

$$\frac{\partial}{\partial\Psi^*_{E'}(x_1,x_2)}\langle E'|\hat{H} - E|E\rangle = 0. \tag{19}$$

With the help of relation in Eq. (17), we find that

$$\hat{H}_{\rm eff}\Psi_E(x_1,x_2) = E\Psi_E(x_1,x_2), \tag{20}$$

where the effective two-particle Hamiltonian is given by the sum of kinetic terms of particle in the trap and interaction potential between two particles:

$$\hat{H}_{\rm eff} = \hat{H}_{\rm trap} + V(x_1 - x_2), \tag{21}$$

where

$$\hat{H}_{\rm trap} = -\frac{1}{2m}\frac{d^2}{dx_1^2} + U(x_1) - \frac{1}{2m}\frac{d^2}{dx_2^2} + U(x_2). \tag{22}$$

In the basis of single particle wave functions, the eigenenergy and eigenstate can be solved by diagonalizing the matrix element of an effective two-particle Hamiltonian,

$$[\hat{H}_{\rm eff}]_{n_1,n_2;n'_1,n'_2} = \delta_{n'_1,n_1}\delta_{n'_2,n_2}(\epsilon^{(0)}_{n_1} + \epsilon^{(0)}_{n_2}) + V_{n_1,n_2;n'_1,n'_2}. \tag{23}$$

3. Separation of center of mass and relative motions

The c.m. motion can be separated out rather straightforwardly for some commonly used traps, such as periodic box in lattice QCD, harmonic oscillator trap in nuclear physics, etc.

$$\hat{H}_{\rm trap} = -\frac{1}{2M}\frac{d^2}{dR^2} + U_{\rm c.m.}(R) - \frac{1}{2\mu}\frac{d^2}{dr^2} + U_{\rm rel}(r), \tag{24}$$

where

$$M = 2m \quad \text{and} \quad \mu = \frac{m}{2}$$

are the total mass and reduced mass of two-particle system, respectively, and

$$R = \frac{x_1 + x_2}{2} \quad \text{and} \quad r = x_1 - x_2$$

are center of mass and relative coordinates of two particles, respectively. The $U_{\rm c.m.}(R)$ and $U_{\rm rel}(r)$ represent the trap potentials for center of mass and relative motions, respectively. As a specific example, the harmonic oscillator trap potential for an individual particle is

$$U(x) = \frac{1}{2}m\omega^2 x^2, \tag{25}$$

where ω is angular frequency of harmonic oscillator. The trap potentials for center of mass and relative motions have the similar forms but the mass of particle, m, must be replaced by total mass and reduced mass, respectively,

$$U_{\rm c.m.}(R) = \frac{1}{2} M\omega^2 R^2, \qquad U_{\rm rel}(r) = \frac{1}{2}\mu\omega^2 r^2. \tag{26}$$

The total wave function is thus the product of center of mass wave function and relative wave function,

$$\Psi_E(x_1, x_2) = \psi^{(\rm c.m.)}_{E_{\rm c.m.}}(R)\psi^{(\rm rel)}_{\epsilon}(r), \qquad E = E_{\rm c.m.} + \epsilon, \tag{27}$$

they satisfy Schrödinger equations:

$$\left[-\frac{1}{2M}\frac{d^2}{dR^2} + U_{\rm c.m.}(R)\right]\psi^{(\rm c.m.)}_{E_{\rm c.m.}}(R) = E_{\rm c.m}\psi^{(\rm c.m.)}_{E_{\rm c.m.}}(R), \tag{28}$$

and

$$\left[-\frac{1}{2\mu}\frac{d^2}{dr^2} + U_{\rm rel}(r) + V(r)\right]\psi^{(\rm rel)}_{\epsilon}(r) = \epsilon\psi^{(\rm rel)}_{\epsilon}(r). \tag{29}$$

C. Two fermions correlation function

In lattice QCD, particles interaction are usually studied via evaluating time dependence of correlation functions numerically from the first principle. To illustrate how the two-particle correlation function is related to a particle scattering phase shift, first we define the forward time propagating two-particle correlation function by

$$C(rt; r'0)|_{t>0} = \theta(t)\langle 0|\hat{\mathcal{O}}_H(r,t)\hat{\mathcal{O}}^\dagger_H(r',0)|0\rangle. \tag{30}$$

The two-particle creation operator in Heisenberg picture is given by

$$\hat{\mathcal{O}}^\dagger_H(r,t) = e^{i\hat{H}t}\hat{\mathcal{O}}^\dagger(r)e^{-i\hat{H}t}, \tag{31}$$

where

$$\hat{\mathcal{O}}^\dagger(r) = \int dR\psi^{(\rm c.m.)}_{E_{\rm c.m.}}(R)\frac{\hat{\psi}^\dagger_\uparrow(x_1)\hat{\psi}^\dagger_\downarrow(x_2) - \hat{\psi}^\dagger_\downarrow(x_1)\hat{\psi}^\dagger_\uparrow(x_2)}{2}, \tag{32}$$

and c.m. motion has been projected out in definition of $\hat{\mathcal{O}}^\dagger(r)$ operator.

Inserting complete energy basis in between two-particle annihilation and creation operators,

$$\sum_E |E\rangle\langle E| = 1,$$

and also using Eq. (11), it is straightforward to show that

$$\langle E|\hat{\mathcal{O}}^\dagger(r)|0\rangle = \psi^{(\rm rel)*}_{\epsilon}(r). \tag{33}$$

We thus find

$$C(rt; r'0)|_{t>0} = e^{-iE_{\rm c.m.}t}C^{(\rm rel)}(rt; r'0)|_{t>0}, \tag{34}$$

where the correlation function for the relative motion of two-particle system is given by

$$C^{(\rm rel)}(rt; r'0)|_{t>0} = \theta(t)\sum_\epsilon e^{-i\epsilon t}\psi^{(\rm rel)}_\epsilon(r)\psi^{(\rm rel)*}_\epsilon(r'). \tag{35}$$

Using identity

$$i\int_{-\infty}^{\infty}\frac{dE}{2\pi}\frac{e^{-iEt}}{E + i0} = \theta(t), \tag{36}$$

the two-particle correlation function can also be written as

$$C^{(\rm rel)}(rt; r'0)|_{t>0} = i\int_{-\infty}^{\infty}\frac{d\lambda}{2\pi}\sum_\epsilon\frac{\psi^{(\rm rel)}_\epsilon(r)\psi^{(\rm rel)*}_\epsilon(r')}{\lambda - \epsilon + i0}e^{-i\lambda t}. \tag{37}$$

Hence the two-particle correlation function is related to Green's function of two-particle interaction in a trap by

$$C^{(\rm rel)}(rt; r'0)|_{t>0} = i\int_{-\infty}^{\infty}\frac{d\lambda}{2\pi}G^{(\rm trap)}(r, r'; \lambda + i0)e^{-i\lambda t}, \tag{38}$$

where the spectral representation of two-particle Green's function is given by

$$G^{(\rm trap)}(r, r'; \lambda) = \sum_\epsilon\frac{\psi^{(\rm rel)}_\epsilon(r)\psi^{(\rm rel)*}_\epsilon(r')}{\lambda - \epsilon}, \tag{39}$$

and it satisfies the differential equation

$$\left[\epsilon + \frac{1}{2\mu}\frac{d^2}{dr^2} - U_{\rm rel}(r) - V(r)\right]G^{(\rm trap)}(r, r'; \epsilon) = \delta(r - r'). \tag{40}$$

III. INTEGRATED TWO-PARTICLE CORRELATION FUNCTION AND ITS RELATION TO SCATTERING PHASE SHIFT

The detailed derivation of how an integrated two-particle correlation function is related to scattering phase shift are presented in Sec. III B, we show that the infinite volume limit of difference of integrated correlation functions between two interacting and noninteracting particles in the trap approaches

$$\frac{1}{\pi}\int_0^\infty d\epsilon\frac{d\delta(\epsilon)}{d\epsilon}e^{-i\epsilon t} + \frac{\delta(0)}{\pi},$$

where $\delta(\epsilon)$ is a two-particle scattering phase shift in infinite volume. The relation is then illustrated by using an exactly solvable contact interaction model in both periodic box and harmonic oscillator trap in Sec. III C.

A. Integrated two-particle correlation function

Using orthogonality of two-particle wave function, the integrated two-particle correlation function is related to energy spectra simply by

$$C^{(\mathrm{rel})}(t)|_{t>0} = \int dr C^{(\mathrm{rel})}(rt; r0)|_{t>0} = \theta(t) \sum_{\epsilon} e^{-i\epsilon t}. \quad (41)$$

Using Eq. (38), the integrated two-particle correlation function is therefore also given by

$$C^{(\mathrm{rel})}(t)|_{t>0} = i \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} \mathrm{Tr}[G^{(\mathrm{trap})}(\lambda + i0)] e^{-i\lambda t}, \quad (42)$$

where the trace of Green's function is defined by

$$\mathrm{Tr}[G^{(\mathrm{trap})}(\lambda)] = \int dr G^{(\mathrm{trap})}(r, r; \lambda). \quad (43)$$

B. Relating integrated correlation function to scattering phase shift

1. Quantization condition of energy spectra in a trap and infinite volume limit of integrated correlation function

With a short-range interaction, the quantization condition (QC) that determines discrete energy spectra of the trapped two-particle system can be formulated in a compact form, for instance, Lüscher formula [4] in a periodic cubic box in LCQD and BERW formula [5] in a harmonic oscillator trap in nuclear physics,

$$\det\left[\cot \delta(\epsilon) - \mathcal{M}(\epsilon)\right] = 0, \quad (44)$$

where $\delta(\epsilon)$ refers to the diagonal matrix of scattering partial wave phase shifts, and the matrix function $\mathcal{M}(\epsilon)$ is associated to the geometry and dynamics of trap itself. Lüscher and BERW formula both are the result of presence of two well separated physical scales: (1) short-range interaction between two particles and (2) size of trap. Therefore the short-range dynamics that is described by scattering phase shift and long-range correlation effect due to the trap can be factorized, also see recent developments and extension of Lüscher and BERW formalism beyond two-particle sector and elastic region, Refs. [6–45].

For a particular partial wave state, Eq. (44) can be rearranged to

$$\delta_l(\epsilon) + \phi_l(\epsilon) = n\pi, \qquad n \in \mathbb{Z}, \quad (45)$$

where l stands for the angular momentum of system. The expression of $\phi_l(\epsilon)$ is associated to matrix elements of $\mathcal{M}(\epsilon)$ and may depends on other partial wave phase shifts as well. For example, in BERW formula with a harmonic oscillator trap, see, e.g., Refs. [5,35], the rotational symmetry is well preserved, so $[\mathcal{M}(\epsilon)]_{l,l'} = \delta_{l,l'} \mathcal{M}_l(\epsilon)$, and $\phi_l(\epsilon) = -\cot^{-1}[\mathcal{M}_l(\epsilon)]$ is totally determined by the diagonal element of a $\mathcal{M}(\epsilon)$ matrix. However in a periodic cubic box, see, e.g., Refs. [4,35], the rotational symmetry is broken and angular orbital momenta are no longer good quantum numbers; hence $\mathcal{M}(\epsilon)$ in general is not a diagonal matrix. $\phi_l(\epsilon)$ now not only depends on the matrix element of $\mathcal{M}(\epsilon)$, but it also depends on other partial wave phase shifts as well.

In one-dimensional space, partial wave angular momentum states are replaced by the parity states. In our case, for spin singlet two-fermion states, only even parity state contributes, so from this point on, the subscript-l in Eq. (45) will be dropped, the quantization condition is simply written as

$$\delta(\epsilon_n) + \phi(\epsilon_n) = n\pi, \quad (46)$$

where subscript-n in ϵ_n is used to label the nth eigenenergy of system. The analytic expression of $\phi(\epsilon)$ for a periodic box and h.o. trap are given in Appendix A, respectively, by

$$\phi(\epsilon) = \begin{cases} \sqrt{2\mu\epsilon}\frac{L}{2}, & \text{for a periodic box} \\ -\cot^{-1}\left[\sqrt{\frac{\epsilon}{2\omega}} \frac{\Gamma(\frac{1}{4} - \frac{\epsilon}{2\omega})}{\Gamma(\frac{3}{4} - \frac{\epsilon}{2\omega})}\right], & \text{for a h.o. trap} \end{cases}, \quad (47)$$

where L stands for the size of periodic box, so that the wave function in c.m. frame with zero total momentum satisfies periodic boundary condition of

$$\psi_{\epsilon}^{(\mathrm{rel})}(r + nL) = \psi_{\epsilon}^{(\mathrm{rel})}(r), \qquad n \in \mathbb{Z}. \quad (48)$$

The technical details of derivation of Eq. (47) can be found in Refs. [31,33,34] and also Appendix A, the same approach applies to the one-dimensional case as well.

Using the fact that

$$\frac{1}{\pi}[\triangle\delta(\epsilon_n) + \triangle\phi(\epsilon_n)] = 1, \quad n = 0, 1, \ldots, \quad (49)$$

where

$$\triangle\delta(\epsilon_n) = \delta(\epsilon_{n+1}) - \delta(\epsilon_n), \qquad \triangle\phi(\epsilon_n) = \phi(\epsilon_{n+1}) - \phi(\epsilon_n), \quad (50)$$

we thus have a relation

$$\sum_{n=0}^{\infty} e^{-i\epsilon_n t} = \frac{1}{\pi} \sum_{n=0}^{\infty} \triangle\epsilon_n \left[\frac{\triangle\delta(\epsilon_n)}{\triangle\epsilon_n} + \frac{\triangle\phi(\epsilon_n)}{\triangle\epsilon_n}\right] e^{-i\epsilon_n t}, \quad (51)$$

where $\triangle\epsilon_n = \epsilon_{n+1} - \epsilon_n$. When the particle interaction is turned off, $\delta(\epsilon) \to 0$, the energy spectra is totally determined by condition

$$\phi(\epsilon_n^{(0)}) = n\pi,$$

where $\epsilon_n^{(0)}$ stands for the nth eigenenergy of noninteracting two-fermion system in a trap. Hence, we also have a relation,

$$\sum_{n=0}^{\infty} e^{-i\epsilon_n^{(0)} t} = \frac{1}{\pi}\sum_{n=0}^{\infty} \triangle\epsilon_n^{(0)} \frac{\triangle\phi(\epsilon_n^{(0)})}{\triangle\epsilon_n^{(0)}} e^{-i\epsilon_n^{(0)} t}. \quad (52)$$

As the system in a trap is approaching infinite volume limit, such as $L \to \infty$ in a periodic box or $\omega \to 0$ in a harmonic oscillator trap, we find

$$\sum_{n=0}^{\infty} e^{-i\epsilon_n t} \overset{\text{trap}\to\infty}{\to} \frac{1}{\pi}\int_0^\infty d\epsilon \left[\frac{d\delta(\epsilon)}{d\epsilon} + \frac{d\phi(\epsilon)}{d\epsilon}\right] e^{-i\epsilon t} \quad (53)$$

and

$$\sum_{n=0}^{\infty} e^{-i\epsilon_n^{(0)} t} \overset{\text{trap}\to\infty}{\to} \frac{1}{\pi}\int_0^\infty d\epsilon \frac{d\phi(\epsilon)}{d\epsilon} e^{-i\epsilon t}. \quad (54)$$

Hence it is tempting to conclude that

$$\sum_{n=0}^{\infty} \left[e^{-i\epsilon_n t} - e^{-i\epsilon_n^{(0)} t}\right] \overset{\text{trap}\to\infty}{\to} \frac{1}{\pi}\int_0^\infty d\epsilon \frac{d\delta(\epsilon)}{d\epsilon} e^{-i\epsilon t}. \quad (55)$$

At the limit of $V(r) \to 0$, the left-hand side of Eq. (55) clearly approaches zero, on the contrary, on the right-hand side of Eq. (55), the weak interaction limit of $\frac{d\delta(\epsilon)}{d\epsilon}$ is not always well defined, such as in the case of 1D contact interaction potential. However, in general, the weak interaction limit of $\delta(\epsilon)$ is well defined and approaches zero; hence, using integration by part, we find

$$\frac{1}{\pi}\int_0^\infty d\epsilon \frac{d\delta(\epsilon)}{d\epsilon} e^{-i\epsilon t} \overset{V(r)\to 0}{\to} -\frac{\delta(0)}{\pi}, \quad (56)$$

where $\delta(0)$ is the possible nontrivial surface term as the result of integration by part, other surface terms are assumed trivial and vanishing. For instance, for the particles interacting with a contact interaction in 1D, the phase shift at branch point has nontrivial value: $\delta(0) = -\frac{\pi}{2}$. In order to make sure both sides of Eq. (55) approach zero at the limit of weak interaction, the constant shift, $-\frac{\delta(0)}{\pi}$, at right-hand side must be subtracted. Therefore, at the infinite volume limit, the difference between integrated correlation functions with and without particle interactions is associated to scattering phase shift by

$$[C^{(\text{rel})}(t) - C_0^{(\text{rel})}(t)]_{t>0} \overset{\text{trap}\to\infty}{\to} \frac{\theta(t)}{\pi}\int_0^\infty d\epsilon \frac{d\delta(\epsilon)}{d\epsilon} e^{-i\epsilon t} + \frac{\theta(t)}{\pi}\delta(0), \quad (57)$$

where $C_0^{(\text{rel})}(t)$ is the integrated correlation function of noninteracting particles in a trap,

$$C_0^{(\text{rel})}(t)|_{t>0} = \theta(t)\sum_{n=0}^{\infty} e^{-i\epsilon_n^{(0)} t}. \quad (58)$$

Similarly, the constant shift, $-\frac{\delta(0)}{\pi}$, must be subtracted in Eq. (53) as well

$$\sum_{n=0}^{\infty} e^{-i\epsilon_n t} \overset{\text{trap}\to\infty}{\to} \frac{1}{\pi}\int_0^\infty d\epsilon \left[\frac{d\delta(\epsilon)}{d\epsilon} + \frac{d\phi(\epsilon)}{d\epsilon}\right] e^{-i\epsilon t} + \frac{\delta(0)}{\pi}. \quad (59)$$

2. The role of Friedel formula and Krein's theorem

The expression in Eq. (57) can also be understood by the relation displayed in Eq. (42). In terms of Green's function of a two-particle system in the trap, the difference between integrated correlation functions with and without particle interactions is also given by

$$\left[C^{(\text{rel})}(t) - C_0^{(\text{rel})}(t)\right]_{t>0} = i\int_{-\infty}^{\infty} \frac{d\lambda}{2\pi}\left[\text{Tr}[G^{(\text{trap})}(\lambda + i0) - G_0^{(\text{trap})}(\lambda + i0)]\right] e^{-i\lambda t}, \quad (60)$$

where $\text{Tr}[G_0^{(\text{trap})}(\lambda + i0)]$ stands for the trace of Green's function of two noninteracting particles in the trap. As the system is approaching infinite volume limit, thus

$$\left[C^{(\text{rel})}(t) - C_0^{(\text{rel})}(t)\right]_{t>0} \overset{\text{trap}\to\infty}{\to} i\int_{-\infty}^{\infty} \frac{d\lambda}{2\pi}\left[\text{Tr}[G^{(\infty)}(\lambda + i0) - G_0^{(\infty)}(\lambda + i0)]\right] e^{-i\lambda t}. \quad (61)$$

As demonstrated in Refs. [64–68] and also see discussion in Ref. [69], the difference between the trace of Green's function of the interacting system and free particle system is related to the scattering phase shift by Friedel formula and Krein's theorem, see the short summary in Appendix B,

$$-\text{Tr}[G^{(\infty)}(\lambda) - G_0^{(\infty)}(\lambda)] = \frac{1}{\pi}\int_0^\infty d\epsilon \frac{\delta(\epsilon)}{(\epsilon - \lambda)^2}, \quad (62)$$

where we have assumed $\text{Tr}[G^{(\infty)}(\lambda)]$ only has a dominant physical branch cut along positive real axis in complex λ plane: $\lambda \in [0, \infty]$ and an unphysical branch cut sitting along a negative real axis has been neglected at the scope of current work. By using Eqs. (62) and (61) thus can be rearranged to

$$\left[C^{(\mathrm{rel})}(t) - C_0^{(\mathrm{rel})}(t)\right]_{t>0} \overset{\mathrm{trap}\to\infty}{\to} -\frac{1}{\pi}\int_0^\infty d\epsilon\delta(\epsilon)\frac{d}{d\epsilon} \times \left[i\int_{-\infty}^{\infty}\frac{d\lambda}{2\pi}\frac{e^{-i\lambda t}}{\lambda-\epsilon+i0}\right]. \tag{63}$$

Using the identity Eq. (36) again, we find

$$\left[C^{(\mathrm{rel})}(t) - C_0^{(\mathrm{rel})}(t)\right]_{t>0} \overset{\mathrm{trap}\to\infty}{\to} -\frac{\theta(t)}{\pi}\int_0^\infty d\epsilon\delta(\epsilon)\frac{de^{-i\epsilon t}}{d\epsilon}, \tag{64}$$

hence by integrating by part and assuming $\delta(\infty)\to 0$, Eq. (57) is obtained again.

C. One-dimensional analytic solutions of two fermions in traps interacting with a contact interaction

In this subsection, the infinite volume limit of difference of integrated correlation functions between two interacting and noninteracting particles in the trap is illustrated by considering a simple contact interaction model. The scattering phase shift of particles interaction in infinite volume is exactly solvable. Both a periodic box and a harmonic oscillator trap are considered; the derivation of analytic expression of quantization conditions in both cases are presented in Appendix A. The discrete energy spectra of particles interaction in a trap can be solved rather straightforwardly numerically. We will show that the difference of integrated correlation functions in both cases approaches the same infinite volume limit that is solely determined by particles interaction steadily and converge rather fast near small t region.

1. Periodic box

Let us first consider a simple problem of 1D two-fermion of total spin-zero interacting with a contact interaction in a periodic box, the dynamics of the two-particle system in a c.m. frame is described by

$$\left[-\frac{1}{2\mu}\frac{d^2}{dr^2} + V_0\sum_{n\in\mathbb{Z}}\delta(r+nL)\right]\psi_\epsilon^{(\mathrm{rel})}(r) = \epsilon\psi_\epsilon^{(\mathrm{rel})}(r), \tag{65}$$

where V_0 is the strength of contact interaction and L is the size of periodic box. The wave function is symmetric under spatial inversion, $\psi_\epsilon^{(\mathrm{rel})}(-r) = \psi_\epsilon^{(\mathrm{rel})}(r)$, and also must satisfy the periodic boundary condition in Eq. (48). For a contact interaction, the analytic expression of quantization condition can be obtained, see, e.g., Refs. [20–23],

$$\delta(\epsilon_n) + \sqrt{2\mu\epsilon_n}\frac{L}{2} = n\pi, \qquad n = 0, 1, \ldots, \tag{66}$$

where the analytic expression of phase shift is

$$\delta(\epsilon) = \cot^{-1}\left(-\frac{\sqrt{2\mu\epsilon}}{\mu V_0}\right). \tag{67}$$

The integrated correlation function of trapped system in Euclidean time, $t=-i\tau$, is defined by

$$C^{(\mathrm{rel})}(t) - C_0^{(\mathrm{rel})}(t) \overset{t=-i\tau}{=} \sum_{n=0}^{\infty}\left[e^{-\epsilon_n\tau} - e^{-\epsilon_n^{(0)}\tau}\right], \tag{68}$$

where the energy spectra of interacting trapped system, ϵ_n, are determined by Eq. (66), see, e.g., Fig. 1(a).

$$\epsilon_n^{(0)} = \frac{1}{2\mu}\left(\frac{2\pi n}{L}\right)^2$$

is energy spectrum of noninteracting particles in a periodic box. $C_0^{(\mathrm{rel})}(t)$ can be evaluated analytically,

$$C_0^{(\mathrm{rel})}(t) \overset{t=-i\tau}{=} \frac{1}{2} + \frac{1}{2}\vartheta_3(e^{-(\frac{2\pi}{L})^2\frac{\tau}{2\mu}}) \overset{L\to\infty}{\to} \sqrt{\frac{\mu}{2\pi\tau}}\frac{L}{2}, \tag{69}$$

where $\vartheta_3(z)$ is Jacobi elliptic theta function [70]. At the limit of large volume, according to Eq. (59), we also have

$$\sum_{n=0}^{\infty} e^{-\epsilon_n\tau} \underset{t=-i\tau}{\overset{L\to\infty}{\to}} \frac{1}{\pi}\int_0^\infty d\epsilon\left[\frac{d\delta(\epsilon)}{d\epsilon} + \frac{\mu}{\sqrt{2\mu\epsilon}}\frac{L}{2}\right]e^{-\epsilon\tau} + \frac{\delta(0)}{\pi}. \tag{70}$$

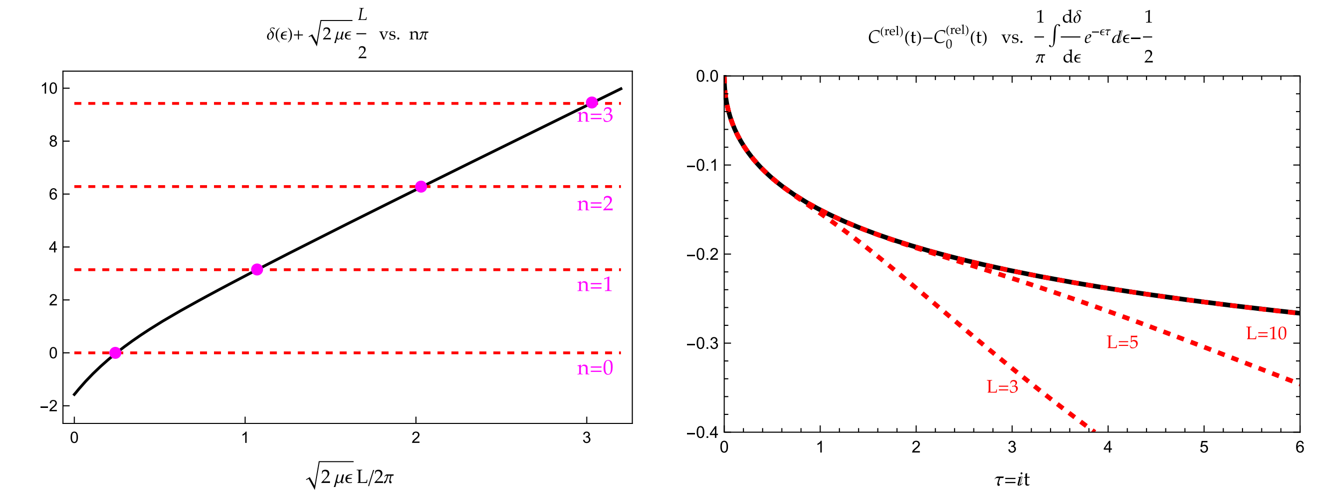
Using Eq. (67), the analytic expression on the right-hand side of above equation can be obtained

$$C^{(\mathrm{rel})}(t) \underset{t=-i\tau}{\overset{L\to\infty}{\to}} \frac{1}{2}\mathrm{erfc}\left(\mu V_0\sqrt{\frac{\tau}{2\mu}}\right)e^{(\mu V_0)^2\frac{\tau}{2\mu}} + \sqrt{\frac{\mu}{2\pi\tau}}\frac{L}{2} - \frac{1}{2}. \tag{71}$$

We can now see clearly that both $C_0^{(\mathrm{rel})}(t)$ and $C^{(\mathrm{rel})}(t)$ have the same divergent behavior, $\sqrt{\frac{\mu}{2\pi\tau}}\frac{L}{2}$, at the limit of $L\to\infty$ and also $\tau\to 0$. However, the divergence cancel out completely between them; hence we find

$$C^{(\mathrm{rel})}(t) - C_0^{(\mathrm{rel})}(t) \underset{t=-i\tau}{\overset{L\to\infty}{\to}} \frac{1}{2}\mathrm{erfc}\left(\mu V_0\sqrt{\frac{\tau}{2\mu}}\right)e^{(\mu V_0)^2\frac{\tau}{2\mu}} - \frac{1}{2}, \tag{72}$$

see Fig. 1(b) for the comparison of difference of integrated correlation functions in a periodic box vs infinite volume limit.



(a) (b)

FIG. 1. The energy spectra and difference of integrated correlation function plots for particles interaction in a periodic box: (a) $\delta(\epsilon_n) + \sqrt{2\mu\epsilon_n}\frac{L}{2}$ (solid black) vs $n\pi$ (dashed red) with $L = 3$, energy spectra are located at intersection points of black and red curves; (b) $\frac{1}{\pi}\int_0^\infty d\epsilon \frac{d\delta(\epsilon)}{d\epsilon} e^{-\epsilon\tau} - \frac{1}{2}$ (solid black) vs $C^{(\mathrm{rel})}(t) - C_0^{(\mathrm{rel})}(t)$ (dashed red) with $L = 3, 5, 10$. The rest of parameters are taken as $V_0 = 0.5$ and $\mu = 1$.

2. *Harmonic oscillator trap*

Next let us consider two fermions of zero total spin interacting by a contact potential in a harmonic oscillator trap, the dynamics of two-particle system is described by

$$\left[-\frac{1}{2\mu}\frac{d^2}{dr^2} + \frac{1}{2}\mu\omega^2 r^2 + V_0\delta(r)\right]\psi_\epsilon^{(\mathrm{rel})}(r) = \epsilon\psi_\epsilon^{(\mathrm{rel})}(r). \quad (73)$$

The spatial wave function again must be symmetric under spatial inversion, $\psi_\epsilon^{(\mathrm{rel})}(-r) = \psi_\epsilon^{(\mathrm{rel})}(r)$, then only even-parity solutions will contribute to the difference of integrated correlation functions. The analytic expression of QC is still given by, see, e.g., Refs. [33,34],

$$\delta(\epsilon_n) + \phi(\epsilon_n) = n\pi,$$

where $\phi(\epsilon)$ is assumed a smooth monotonically varying function,

$$\phi(\epsilon) = -\cot^{-1}\left[\sqrt{\frac{\epsilon}{2\omega}}\frac{\Gamma(\frac{1}{4} - \frac{\epsilon}{2\omega})}{\Gamma(\frac{3}{4} - \frac{\epsilon}{2\omega})}\right] + l\pi, \qquad l \in \mathbb{Z}. \quad (74)$$

The $l\pi$ is added to keep $\phi(\epsilon)$ monotonically when $\cot^{-1}(z)$ starts jumping between branches, see, e.g., Fig. 2(a). Asymptotically $\phi(\epsilon)$ thus behaves as

$$\phi(\epsilon) \overset{\omega\to 0}{\to} \begin{cases} \pi(\frac{\epsilon}{2\omega} - \frac{1}{4}), & \epsilon \gg \omega \\ -\frac{\pi}{2} + \frac{\Gamma[\frac{1}{4}]}{\Gamma[\frac{3}{4}]}\sqrt{\frac{\epsilon}{2\omega}}, & \epsilon \ll \omega \end{cases}. \quad (75)$$

The noninteracting energy spectra of h.o. trap are

$$\epsilon_n^{(0)} = \omega\left(n + \frac{1}{2}\right);$$

hence for even parity solutions, we have

$$\sum_{n=0}^{\infty} e^{-\omega(2n+\frac{1}{2})\tau} = \frac{1}{2}\mathrm{csch}(\omega\tau)e^{\frac{\omega\tau}{2}} \overset{\omega\to 0}{\to} \frac{1}{2\omega\tau}. \quad (76)$$

Using asymptotic form of $\phi(\epsilon)$ in Eq. (75), we find

$$\frac{1}{\pi}\int_0^\infty d\epsilon \frac{d\phi(\epsilon)}{d\epsilon}e^{-\epsilon\tau} \simeq \frac{1}{\pi}\int_0^\omega d\epsilon \frac{d\phi(\epsilon)}{d\epsilon}e^{-\epsilon\tau} + \frac{e^{-\omega\tau}}{2\omega\tau} \overset{\omega\to 0}{\to} \frac{1}{2\omega\tau} \quad (77)$$

and

$$\sum_{n=0}^{\infty} e^{-\epsilon_n\tau} \overset{\omega\to 0}{\to} \frac{1}{2}\mathrm{erfc}\left(\mu V_0\sqrt{\frac{\tau}{2\mu}}\right)e^{(\mu V_0)^2\frac{\tau}{2\mu}} + \frac{1}{2\omega\tau} - \frac{1}{2}. \quad (78)$$

Similarly in harmonic oscillator trap, both $C_0^{(\mathrm{rel})}(t)$ and $C^{(\mathrm{rel})}(t)$ again show the exact same divergence, $\frac{1}{2\omega\tau}$, at the limit of $\omega \to 0$ and also $\tau \to 0$. Hence after the cancellation of divergence, we find again

$$C^{(\mathrm{rel})}(t) - C_0^{(\mathrm{rel})}(t) \underset{t=-i\tau}{\overset{\omega\to 0}{\to}} \frac{1}{2}\mathrm{erfc}\left(\mu V_0\sqrt{\frac{\tau}{2\mu}}\right)e^{(\mu V_0)^2\frac{\tau}{2\mu}} - \frac{1}{2}, \quad (79)$$

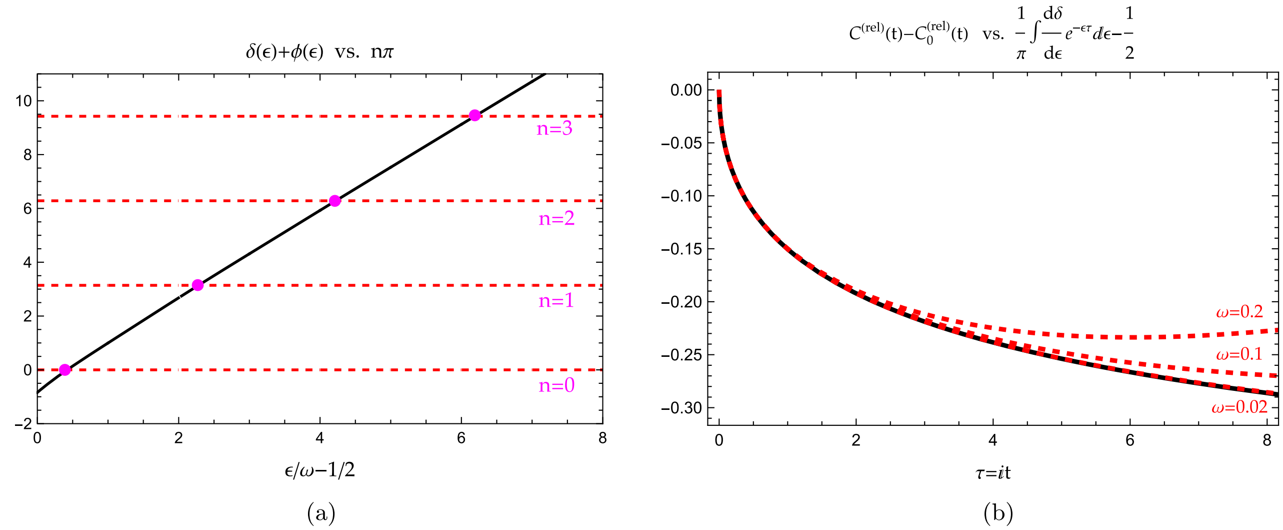


FIG. 2. The energy spectra and difference of integrated correlation function plots for particles interaction in a harmonic oscillator trap: (a) $\delta(\epsilon_n) + \phi(\epsilon_n)$ (solid black) vs $n\pi$ (dashed red) with $\omega = 0.2$, energy spectra are located at intersection points of black and red curves; (b) $\frac{1}{\pi}\int_0^\infty d\epsilon \frac{d\delta(\epsilon)}{d\epsilon} e^{-\epsilon\tau} - \frac{1}{2}$ (solid black) vs $C^{(\mathrm{rel})}(t) - C_0^{(\mathrm{rel})}(t)$ (dashed red) with $\omega = 0.02$, 0.1, 0.2. The rest of parameters are taken as $V_0 = 0.5$ and $\mu = 1$.

see Fig. 2(b) for the comparison of difference of integrated correlation functions in the harmonic oscillator trap vs infinite volume limit.

D. A short summary

Now we can see clearly that, regardless the type of traps that are used, at infinite volume limit where the size of trap is much larger than the range of interactions, the difference of integrated correlation functions of trapped systems all approach the same limit,

$$C^{(\mathrm{rel})}(t) - C_0^{(\mathrm{rel})}(t) \underset{t=-i\tau}{\overset{\mathrm{trap}\to\infty}{\to}} \frac{1}{\pi}\int_0^\infty d\epsilon \frac{d\delta(\epsilon)}{d\epsilon} e^{-\epsilon\tau} + \frac{\delta(0)}{\pi}, \quad (80)$$

where the phase shift is given by

$$\delta(\epsilon) = \cot^{-1}\left(-\frac{\sqrt{2\mu\epsilon}}{\mu V_0}\right)$$

for contact interaction potential. The analytic expression of infinite volume limit is given by

$$\frac{1}{\pi}\int_0^\infty d\epsilon \frac{d\delta(\epsilon)}{d\epsilon} e^{-\epsilon\tau} + \frac{\delta(0)}{\pi} = \frac{1}{2}\mathrm{erfc}\left(\mu V_0\sqrt{\frac{\tau}{2\mu}}\right) e^{(\mu V_0)^2\frac{\tau}{2\mu}} - \frac{1}{2}. \quad (81)$$

As also illustrated in periodic box and harmonic oscillator trap examples, though both $C^{(\mathrm{rel})}(t)$ and $C_0^{(\mathrm{rel})}(t)$ are divergent as $\tau \sim 0$, the divergence is canceled out exactly in the difference of 2, hence $C^{(\mathrm{rel})}(t) - C_0^{(\mathrm{rel})}(t) \overset{\tau\sim 0}{\to} 0$ smoothly.

IV. PERTURBATION CALCULATION OF TWO FERMIONS CORRELATION FUNCTION OF A LATTICE FIELD THEORY MODEL

In this section, we consider a lattice field theory model of fermions interacting with a contact interaction in a periodic box. For the weak interaction coupling strength, the perturbation calculation of two fermions correlation function can be carried out directly in path integral representation. We demonstrated that the infinite volume limit of difference of integrated correlation functions indeed approaches analytic results in Eqs. (80) and (81).

The two fermions correlation function in lattice theory usually is computed in Euclidean space-time by path integral representation,

$$C^{(\mathrm{rel})}(r, t; r', 0) = \frac{\int \mathcal{D}\psi\mathcal{D}\psi^\dagger \hat{O}(r,\tau)\hat{O}^\dagger(r',0) e^{-S_E[\psi,\psi^\dagger]}}{\int \mathcal{D}\psi\mathcal{D}\psi^\dagger e^{-S_E[\psi,\psi^\dagger]}}, \quad (82)$$

where again $t = -i\tau$. The relative motion of two-particle creation operator is projected by

$$\hat{O}^\dagger(r,\tau) = \int_0^L \frac{dx_2}{\sqrt{L}} \frac{\psi_\uparrow^\dagger(r+x_2,\tau)\psi_\downarrow^\dagger(x_2,\tau) - \psi_\downarrow^\dagger(r+x_2,\tau)\psi_\uparrow^\dagger(x_2,\tau)}{2}. \quad (83)$$

The Euclidean action for fermions interacting with a contact interaction in a periodic box with size of L is defined by

$$S_E[\psi,\psi^\dagger] = S_0 + S_V,$$
$$S_0 = \int_{-\infty}^{\infty} d\tau \int_0^L dx \sum_{\sigma=\uparrow,\downarrow} \psi_\sigma^\dagger(x,\tau)\left(\partial_\tau - \frac{\nabla^2}{2m}\right)\psi_\sigma(x,\tau),$$
$$S_V = \frac{V_0}{2}\int_{-\infty}^{\infty} d\tau \int_0^L dx \psi_\uparrow^\dagger(x,\tau)\psi_\uparrow(x,\tau) \times \psi_\downarrow^\dagger(x,\tau)\psi_\downarrow(x,\tau). \quad (84)$$

The fermion field operators satisfy periodic boundary condition,

$$\psi_\sigma(x+L,\tau) = \psi_\sigma(x,\tau), \quad \psi_\sigma^\dagger(x+L,\tau) = \psi_\sigma^\dagger(x,\tau). \quad (85)$$

We remark that in current scope of discussion, zero lattice spacings in both spatial and temporal directions are assumed. The size of lattice extent in temporal direction is also considered infinitely large. Hence lattice artifacts, such as finite lattice spacings and thermal effect in finite lattice size in temporal direction, etc., are avoided in the current discussion. The focus of current work is thus given to the finite volume effect of correlation function of a trapped fermions system in a periodic box and its infinite volume limit.

The complete and analytic solutions of two fermions correlation function in path integral representation in field theory seems like a formidable task in general. Fortunately for the weak interaction, $V_0 \sim 0$, perturbation theory can be carried out. The leading order effect of two fermions correlation function can be obtained rather straightforwardly, and the higher order effects can be carried out systematically in principle. In current work, the only leading order effect of two fermions correlation function is evaluated, and we show that its infinite volume limit indeed is consistent with perturbation expansion of Eq. (81).

A. The leading order effect of perturbation calculation

For weak interaction, $V_0 \sim 0$, two-particle correlation function can be computed analytically by perturbation expansion of

$$e^{-S_E} \sim (1 - S_V + \cdots)e^{-S_0}.$$

The leading order result is thus given by

$$C^{(\mathrm{rel})}(r,t;r',0) - C_0^{(\mathrm{rel})}(r,t;r',0) = -\frac{\int \mathcal{D}\psi\mathcal{D}\psi^\dagger \hat{O}(r,\tau)\hat{O}^\dagger(r',0)S_V e^{-S_0}}{\int \mathcal{D}\psi\mathcal{D}\psi^\dagger e^{-S_0}} + \mathcal{O}(V_0^2). \quad (86)$$

Working out all the Wick contractions, we thus find

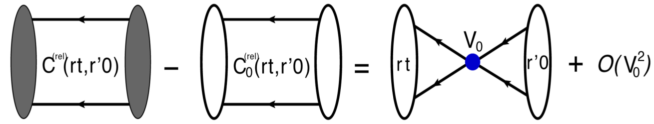


FIG. 3. Diagrammatic representation of perturbation calculation in Eq. (87).

$$C^{(\mathrm{rel})}(r,t;r',0) - C_0^{(\mathrm{rel})}(r,t;r',0) = -\frac{V_0}{L}\int_0^L dx_2 \int_0^L dx_2' \int_{-\infty}^{\infty} d\tau'' \int_0^L dx'' \times D_0^{-1}(r+x_2-x'',\tau-\tau'')D_0^{-1}(x_2-x'',\tau-\tau'') \times D_0^{-1}(x''-r'-x_2',\tau'')D_0^{-1}(x''-x_2',\tau'') + \mathcal{O}(V_0^2), \quad (87)$$

where a free single fermion propagator is defined by

$$\delta_{\sigma,\sigma'}D_0^{-1}(x-x',\tau-\tau') = \frac{\int \mathcal{D}\psi\mathcal{D}\psi^\dagger \psi_\sigma(x,\tau)\psi_{\sigma'}^\dagger(x',\tau')e^{-S_0}}{\int \mathcal{D}\psi\mathcal{D}\psi^\dagger e^{-S_0}}. \quad (88)$$

The diagrammatic representation of Eq. (87) is illustrated in Fig. 3.

Using S_0 in Eq. (84), and the Fourier expansion of a free fermion field operator in Euclidean space-time,

$$\psi_\sigma(x,\tau) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{1}{L}\sum_{k=\frac{2\pi n}{L},n\in\mathbb{Z}} e^{i\omega\tau}e^{ikx}\tilde{\psi}_\sigma(k,\omega), \quad (89)$$

the free single fermion propagator can be worked out rather straightforwardly, and we find

$$D_0^{-1}(x-x',\tau-\tau') = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{1}{L}\sum_{k=\frac{2\pi n}{L},n\in\mathbb{Z}} \frac{e^{i\omega(\tau-\tau')}e^{ik(x-x')}}{i\omega + \frac{k^2}{2m}}. \quad (90)$$

Therefore we also find

$$C^{(\mathrm{rel})}(r,t;r',0) - C_0^{(\mathrm{rel})}(r,t;r',0) = -V_0\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{i\omega\tau}G_0^{(L)}(r;-i\omega)G_0^{(L)}(r';-i\omega), \quad (91)$$

where two-fermion Green's function in a periodic box is defined by

$$G_0^{(L)}(r;-i\omega) = \frac{1}{L}\sum_{k=\frac{2\pi n}{L},n\in\mathbb{Z}} \frac{e^{ikr}}{-i\omega - \frac{k^2}{2\mu}}, \quad (92)$$

the analytic expression of $G_0^{(L)}$ function is given by Eq. (A6).

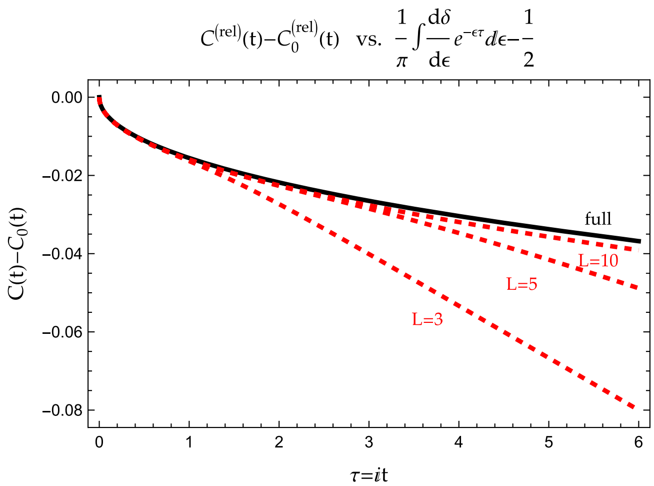


FIG. 4. Perturbation calculation of $C^{(\mathrm{rel})}(t)-C_0^{(\mathrm{rel})}(t)$ (dashed red) with $L=3$, 5, 10 vs full result in infinite volume limit $\frac{1}{\pi}\int_0^\infty d\epsilon \frac{d\delta(\epsilon)}{d\epsilon}e^{-\epsilon\tau}-\frac{1}{2}$ (solid black). The rest of parameters are taken as $V_0=0.04$ and $\mu=1$.

B. Integrated two-fermion correlation function and its infinite volume limit

With perturbation result in Eq. (91), the difference of integrated two-fermion correlation function

$$C^{(\mathrm{rel})}(t)-C_0^{(\mathrm{rel})}(t)=\int_0^L[C^{(\mathrm{rel})}(r,t;r,0)-C_0^{(\mathrm{rel})}(r,t;r,0)], \tag{93}$$

is thus given by

$$C^{(\mathrm{rel})}(t)-C_0^{(\mathrm{rel})}(t)=V_0\sum_{k=\frac{2\pi n}{L},n\in\mathbb{Z}}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{i\omega\tau}\times\frac{d}{d(i\omega)}\left(\frac{1}{i\omega+\frac{k^2}{2\mu}}\right), \tag{94}$$

the integration of ω can be carried out by integration by part, we thus find

$$C^{(\mathrm{rel})}(t)-C_0^{(\mathrm{rel})}(t)=-\tau\frac{V_0}{L}\vartheta_3(e^{-(\frac{2\pi}{L})^2\frac{\tau}{2\mu}}), \tag{95}$$

where

$$\vartheta_3(e^{-(\frac{2\pi}{L})^2\frac{\tau}{2\mu}})=\sum_{k=\frac{2\pi n}{L},n\in\mathbb{Z}}e^{-\frac{k^2}{2\mu}\tau}$$

is a Jacobi elliptic theta function [70]. As $L\to\infty$, perturbation calculation indeed approach

$$C^{(\mathrm{rel})}(t)-C_0^{(\mathrm{rel})}(t)\underset{t=-i\tau}{\overset{L\to\infty}{\to}}-\tau V_0\int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{-\frac{k^2}{2\mu}\tau}=-V_0\frac{\sqrt{\mu\tau}}{\sqrt{2\pi}}. \tag{96}$$

This is indeed consistent with the perturbation expansion of analytic result in infinite volume limit in Eq. (81),

$$\frac{1}{2}\mathrm{erfc}\left(\mu V_0\sqrt{\frac{\tau}{2\mu}}\right)e^{(\mu V_0)^2\frac{\tau}{2\mu}}-\frac{1}{2}\overset{V_0\to 0}{\to}-V_0\frac{\sqrt{\mu\tau}}{\sqrt{2\pi}}+\mathcal{O}(V_0^2), \tag{97}$$

also see Fig. 4 for an example of the perturbation calculation result vs the full result in infinite volume limit.

C. Leading order contribution of energy levels of two-fermion system in finite volume

As a separate check, we can also evaluate leading order contribution of energy levels of two-fermion system in perturbation theory in finite volume. The individual energy level can be projected out by

$$C^{(\mathrm{rel})}(\tau,\epsilon_n)=\frac{\sigma_n}{L}\int_0^L dr\int_0^L dr' e^{-ik_n(r-r')}C^{(\mathrm{rel})}(r,t;r',0), \tag{98}$$

where $k_n=\frac{2\pi n}{L}$, $n\in\mathcal{Z}$ is the free particle's momentum in finite volume, and $\epsilon_n=\frac{k_n^2}{2\mu}+\delta\epsilon_n$ is the perturbation result of total energy of two fermions system, where $\delta\epsilon_n$ stands for the energy shift due to interaction. The σ_n is degeneracy factor

$$\sigma_n=\begin{cases}2, & \text{if } n>0\\ 1, & \text{if } n=0\end{cases}, \tag{99}$$

since both $k_{\pm n}=\pm k_n$ correspond to the same free two-fermion energy level: $\epsilon_n^{(0)}=\frac{k_n^2}{2\mu}$. The leading order result of energy shift can also be obtained by using quantization condition in Eqs. (66) and (67), up to order of V_0, we thus find

$$\delta\epsilon_n=\sigma_n\frac{V_0}{L}. \tag{100}$$

The same conclusion can be obtained by considering projecting out energy levels from two-fermion correlation function.

First of all, using Eqs. (91) and (98), we thus find

$$C^{(\mathrm{rel})}(\tau,\epsilon_n)-C_0^{(\mathrm{rel})}(\tau,\epsilon_n)=-\tau\frac{\sigma_n V_0}{L}e^{-\frac{k_n^2}{2\mu}\tau}+\mathcal{O}\left(\frac{V_0^2}{L^2}\right), \tag{101}$$

and it is related to Eq. (95) by

$$C^{(\mathrm{rel})}(t) - C_0^{(\mathrm{rel})}(t) = \sum_{n=0}^{\infty}\left[C^{(\mathrm{rel})}(\tau,\epsilon_n) - C_0^{(\mathrm{rel})}(\tau,\epsilon_n)\right]. \tag{102}$$

Next, we also need to consider the free two-fermion correlation function that is defined by

$$C_0^{(\mathrm{rel})}(r,t;r',0) = \frac{\int \mathcal{D}\psi\mathcal{D}\psi^\dagger \hat{O}(r,\tau)\hat{O}^\dagger(r',0)e^{-S_0}}{\int \mathcal{D}\psi\mathcal{D}\psi^\dagger e^{-S_0}} \tag{103}$$

and is given explicitly in terms of free fermion propagators by

$$C_0^{(\mathrm{rel})}(r,t;r',0) = \frac{1}{2L}\int_0^L dx_2 \int_0^L dx_2' \times\left[D_0^{-1}(r+x_2-r'-x_2',\tau)D_0^{-1}(x_2-x_2',\tau) + D_0^{-1}(r+x_2-x_2',\tau)D_0^{-1}(x_2-r'-x_2',\tau)\right]. \tag{104}$$

Using Eq. (88), we thus find

$$C_0^{(\mathrm{rel})}(r,t;r',0) = \frac{1}{L}\sum_{k_n=\frac{2\pi n}{L},n\in\mathbb{Z}} \cos(k_n r)\cos(k_n r')e^{-\frac{k_n^2}{2\mu}\tau}. \tag{105}$$

This is indeed consistent with spectral representation of correlation function in Eq. (35), where the relative wave function of two free particles in a periodic box is given by

$$\psi_{k_n}^{(L)}(r) = \frac{1}{\sqrt{L}}\cos(k_n r), \tag{106}$$

which is normalized by

$$\int_0^L dr \psi_{k_n}^{(L)}(r)\psi_{k_n'}^{(L)*}(r) = \frac{\delta_{k_n,k_n'} + \delta_{k_n,-k_n'}}{2} = \frac{\delta_{|k_n|,|k_n'|}}{\sigma_n}. \tag{107}$$

Hence the projected noninteracting two-fermion correlation function is given by

$$C_0^{(\mathrm{rel})}(\tau,\epsilon_n) = e^{-\frac{k_n^2}{2\mu}\tau}. \tag{108}$$

Putting all together, up to leading order, we find

$$C^{(\mathrm{rel})}(\tau,\epsilon_n) = e^{-\frac{k_n^2}{2\mu}\tau}\left[1 - \tau\frac{\sigma_n V_0}{L} + \mathcal{O}\left(\frac{V_0^2}{L^2}\right)\right]. \tag{109}$$

The leading order contribution of energy level of two-fermion system in a finite volume is therefore obtained by

$$\epsilon_n = -\frac{1}{\tau}\ln C^{(\mathrm{rel})}(\tau,\epsilon_n) = \frac{k_n^2}{2\mu} + \frac{\sigma_n V_0}{L} + \mathcal{O}\left(\frac{V_0^2}{L^2}\right). \tag{110}$$

The leading effect of energy shift due to interaction in a finite volume in perturbation theory is thus again given by $\delta\epsilon_n = \sigma_n \frac{V_0}{L}$.

In terms of perturbation calculation, now we can indeed see the structure mentioned in Eq. (4),

$$C^{(\mathrm{rel})}(t) - C_0^{(\mathrm{rel})}(t) = -\tau\langle\hat{V}(\tau)\rangle + \cdots, \tag{111}$$

where

$$\langle\hat{V}(\tau)\rangle = \sum_{n=0}^{\infty}\left(\frac{\sigma_n V_0}{L}\right)e^{-\epsilon_n^{(0)}\tau} \propto \frac{1}{L}. \tag{112}$$

Also as demonstrated in Fig. 4, the difference of integrated correlation functions approaches infinite volume limit much more rapidly in the region of $\tau \ll L$.

V. MONTE CARLO SIMULATION TEST IN 1D QUANTUM MECHANICS

To demonstrate the feasibility of proposed formalism, we conduct a simple Monte Carlo simulation test with a 1D quantum mechanics model in this section.

A. A 1D quantum mechanics model

Considering a spinless particle with the mass μ interacting with a short-range repulsive square well potential in a harmonic oscillator trap, the eigensolutions are determined by Schrödinger equations,

$$\left[-\frac{1}{2\mu}\frac{d^2}{dr^2} + \frac{1}{2}\mu\omega^2 r^2 + V(r)\right]\psi_n(r) = \epsilon_n\psi_n(r), \tag{113}$$

where

$$V(r) = \begin{cases} \frac{V_0}{b}, & r\in[-\frac{b}{2},\frac{b}{2}] \\ 0, & \text{otherwise} \end{cases}, \quad \overset{b\to 0}{\rightarrow} V_0\delta(r). \tag{114}$$

The energy spectra of the system can be solved by diagonalizing the Hamiltonian matrix

$$H_{n,n'} = \delta_{n,n'}\omega\left(n+\frac{1}{2}\right) + \frac{V_0}{b}\int_{-\frac{b}{2}}^{\frac{b}{2}} dr\varphi_n^{(\omega)*}(r)\varphi_{n'}^{(\omega)}(r), \tag{115}$$

where $\varphi_n^{(\omega)}(r)$ are eigensolutions of harmonic oscillator potential,

$$\varphi_n^{(\omega)}(r) = \frac{1}{\sqrt{2^n n!}}\left(\frac{\mu\omega}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\mu\omega}{2}r^2} H_n(\sqrt{\mu\omega}r). \tag{116}$$

B. Integrated transition amplitude and Monte Carlo simulation

In Euclidean space-time, the transition amplitude for a particle propagating from $(r, 0)$ to (r', τ) is defined by

$$\langle r'|e^{-\hat{H}\tau}|r\rangle = \sum_{n=0}^{\infty} e^{-\epsilon_n \tau} \psi_n(r) \psi_n^*(r'). \tag{117}$$

Hence, integrated transition amplitude (particle propagator) is associated to the partition function in statistics by

$$C(\tau) = \int dr \langle r|e^{-\hat{H}\tau}|r\rangle = \sum_{n=0}^{\infty} e^{-\epsilon_n \tau} \overset{\tau\to\beta}{\to} \mathrm{Tr}[e^{-\beta H}]. \tag{118}$$

The path integral representation of the integrated particle propagator is given by, see, e.g., Refs. [71,72],

$$C(\tau) = \lim_{N_\tau\to\infty} \left(\frac{\mu}{2\pi a_\tau}\right)^{\frac{N_\tau}{2}} \int \prod_{i=1}^{N_\tau} dr_i e^{-S_E(\{r_i\})}, \tag{119}$$

where the time interval $[0, \tau]$ is divided into N_τ small steps of width of $a_\tau = \frac{\tau}{N_\tau}$. The discrete Euclidean space-time action is given by the sum of trap action and interaction term, $S_E(\{r_i\}) = S_E^{(\omega)}(\{r_i\}) + S_E^{(V)}(\{r_i\})$:

$$S_E^{(\omega)}(\{r_i\}) = a_\tau \sum_{i=1}^{N_\tau} \left[\frac{\mu}{2}\left(\frac{r_{i+1} - r_i}{a_\tau}\right)^2 + \frac{1}{2}\mu\omega^2 r_i^2\right] \tag{120}$$

and

$$S_E^{(V)}(\{r_i\}) = a_\tau \sum_{i=1}^{N_\tau} V(r_i), \tag{121}$$

where $r_0 = r$ and $r_{N_\tau} = r' = r$ are initial and finial position of particle, respectively. Similarly when the interaction, $V(r)$, is turned off, the integrated particle propagator in the harmonic oscillator trap is defined by

$$\begin{aligned} C_0(\tau) &= \sum_{n=0}^{\infty} e^{-\omega(n+\frac{1}{2})\tau} = \frac{1}{2}\mathrm{csch}\left(\frac{\omega\tau}{2}\right), \\ &= \lim_{N_\tau\to\infty} \left(\frac{\mu}{2\pi a_\tau}\right)^{\frac{N_\tau}{2}} \int \prod_{i=1}^{N_\tau} dr_i e^{-S_E^{(\omega)}(\{r_i\})}. \end{aligned} \tag{122}$$

For a finite square well model, without the constraint of Pauli exclusive principle, now both even and odd parity states contribute to $C(\tau)$.

The path integral representation of ratio of $C(\tau)$ and $C_0(\tau)$ can be written as

$$\frac{C(\tau)}{C_0(\tau)} = \lim_{N_\tau\to\infty} \int \prod_{i=1}^{N_\tau} dr_i \rho(\{r_i\}) e^{-S_E^{(V)}(\{r_i\})}, \tag{123}$$

where

$$\rho(\{r_i\}) = \left(\frac{\mu}{2\pi a_\tau}\right)^{\frac{N_\tau}{2}} \frac{e^{-S_E^{(\omega)}(\{r_i\})}}{C_0(\tau)} \tag{124}$$

is positive definite and

$$\int \prod_{i=1}^{N_\tau} dr_i \rho(\{r_i\}) = 1. \tag{125}$$

Hence $\rho(\{r_i\})$ can be interpreted as probability density, and Eq. (123) can be computed via a standard Monte Carlo simulation method,

$$\frac{C(\tau)}{C_0(\tau)} = \frac{1}{N_{cfg}} \sum_{\alpha=1}^{N_{cfg}} e^{-S_E^{(V)}(\{r_i^{(\alpha)}\})}, \tag{126}$$

where N_{cfg} is total number of configurations, α is used to label each configuration, the random values of $\{r_i^{(\alpha)}\}$ for each individual configuration can be generated according to the probability density distribution $\rho(\{r_i^{(\alpha)}\})$. The Monte Carlo simulation can be performed rather straightforwardly by standard Metropolis algorithm, see, e.g., Refs. [71,72].

C. Scattering phase shifts and its relation to integrated transition amplitude

The scattering amplitudes for a repulsive square well potential in infinite volume can be solved analytically, see, e.g., Appendix D in Ref. [20]. The phase shifts, $\delta_\pm(\epsilon)$, are given by

$$\delta_\pm(\epsilon) = \cot^{-1}\left[\frac{1 + \left(\frac{k}{k_V}\right)^{\pm 1} \cot\left(\frac{kb}{2}\right) \cot\left(\frac{k_V b}{2}\right)}{\cot\left(\frac{kb}{2}\right) - \left(\frac{k}{k_V}\right)^{\pm 1} \cot\left(\frac{k_V b}{2}\right)}\right], \tag{127}$$

where subscripts $(+/-)$ are used to label even and odd parity states, respectively, and

$$k = \sqrt{2\mu\epsilon}, \qquad k_V = \sqrt{2\mu\left(\epsilon - \frac{V_0}{b}\right)}.$$

As $b \to 0$,

$$\delta_+(\epsilon) \overset{b\to 0}{\to} \cot^{-1}\left(-\frac{k}{\mu V_0}\right), \qquad \delta_-(\epsilon) \overset{b\to 0}{\to} 0, \tag{128}$$

the square well potential approaches a contact interaction, and solutions for odd parity states are suppressed. The scattering phase shifts are associated to $C(\tau)$ and $C_0(\tau)$ by

$$C(\tau) - C_0(\tau) \overset{\omega\to 0}{\to} \frac{1}{\pi}\int_0^\infty d\epsilon \left[\frac{d\delta_+(\epsilon)}{d\epsilon} + \frac{d\delta_-(\epsilon)}{d\epsilon}\right] e^{-\epsilon\tau} + \frac{\delta_+(0) + \delta_-(0)}{\pi}, \tag{129}$$

where $\delta_+(0) = -\frac{\pi}{2}$ and $\delta_-(0) = 0$.

D. Monte Carlo data vs exact solutions vs infinite volume limit result

Numerical test for the system of a spinless particle interacting with a square well potential are carried out and presented in this subsection, the aim is to demonstrate that the Monte Carlo result of a trapped system approaches and converge with infinite volume limit result at small Euclidean time region.

(i) The Monte Carlo computation of $\frac{C(\tau)}{C_0(\tau)}$ in Eq. (126) for the system in a harmonic oscillator trap is carried out by a standard Metropolis algorithm, see, e.g., Refs. [71,72]. The simulations are performed with a fixed number of steps in temporal dimension, $N_\tau = 100$, so the lattice spacing $a_\tau = \frac{\tau}{N_\tau}$ varies for $\tau \in [0.5, 5]$. The typical half million measurements are generated for each τ. The choice of other parameters are $V_0 = 1$, $\mu = 1$, and $b = 0.2$ for a square well potential, and various ωs for a harmonic oscillator trap are used in our simulation: $\omega = 0.1$, 0.2, and 0.5. The variance of data samples are computed by a Jackknife resampling method.

(ii) As a comparison, the energy spectra of particle interacting with a square well potential in a harmonic oscillator trap can be solved by diagonalizing Hamiltonian matrix in Eq. (115), so the exact solution of $\frac{C(\tau)}{C_0(\tau)}$ can be obtained, where $C(\tau) = \sum_{n=0}^{\infty} e^{-\epsilon_n \tau}$ and $C_0(\tau) = \frac{1}{2}\mathrm{csch}(\frac{\omega\tau}{2})$.

(iii) The scattering of a spinless particle off a square well potential in infinite volume can be solved exactly, the analytic expression of phase shifts for both parity states are given in Eq. (127). At infinite volume limit,

$$\frac{C(\tau)}{C_0(\tau)} \overset{\omega\to 0}{\to} 1 + \left[\frac{1}{\pi}\int_0^\infty d\epsilon \frac{d(\delta_+ + \delta_-)}{d\epsilon} e^{-\epsilon\tau} - \frac{1}{2}\right]\omega\tau. \tag{130}$$

For a small $b \sim 0.1$, the scattering solutions of a square well potential agree well with scattering solution of a contact interaction.

The comparison of Monte Carlo data of $\frac{C(\tau)}{C_0(\tau)}$ (red error bars) vs exact solutions (solid black) vs infinite volume limit result (dashed purple) are shown in Figs. 5(a)–5(c) for various ωs. The Monte Carlo data of $C(\tau) - C_0(\tau)$ for various ωs (colored error bars) vs infinite volume limit result (dashed purple) are shown in Fig. 5(d), the infinite volume limit result with a contact interaction (solid blue) is also plotted in Fig. 5(d) as a comparison.

VI. DISCUSSION AND SUMMARY

In summary, a relation between integrated correlation function of a trapped system and infinite volume scattering phase shift is derived in present work. We show that even with a modest size of a trap, the difference of integrated correlation function of a trapped system with and without particle interactions at small Euclidean time region approach steadily to its infinite volume limit that is given in terms of scattering phase shift by

$$C(t) - C_0(t) \underset{t=-i\tau}{\overset{\text{trap}\to\infty}{\to}} \frac{1}{\pi}\int_0^\infty d\epsilon \frac{d\delta(\epsilon)}{d\epsilon} e^{-\epsilon\tau} + \frac{\delta(0)}{\pi}.$$

Therefore, the scattering phase shifts may be extracted from lattice simulation of integrated correlation function at small time region, which is in great contrast to conventional two-step approach in extracting scattering information from lattice calculation: extracting energy levels from temporal correlation function in large Euclidean time region in the first step and then converting energy spectra into phase shifts by applying Lüscher formula in the second step. Both (1) perturbation calculation of $(1+1)$D lattice Euclidean field theory model of fermions interacting with a contact interaction and (2) Monte Carlo simulation of a 1D exactly solvable quantum mechanics model are carried out to explore and test the proposed relation, we show both analytically and numerically that the difference of integrated correlation function of a trapped system indeed agree well with infinite volume limit at small time region even for a modest small size of trap.

The fundamental reason of this observation is due to the fact that integrated trapped correlation functions resemble the partition function in statistical mechanics,

$$C(t) - C_0(t) \overset{t=-i\tau}{\to} \mathrm{Tr}[e^{-\hat{H}\tau} - e^{-\hat{H}_0\tau}],$$

with τ playing the role of the square of the thermal de Broglie wavelength. When thermal de Broglie wavelength is much smaller than size of trap, particles are nearly blind of the size effect of a trap, the difference of integrated trapped two-particle correlation functions can be described in terms of power of τ/L, the leading order contribution is thus proportional to $\tau\langle\hat{V}\rangle$ where $\langle\hat{V}\rangle \sim 1/L$.

The scope of current discussion is still limited to $(1+1)$D nonrelativistic few-particle dynamics. The current focus of this work is to simply demonstrate both numerically and analytically that the difference of integrated trapped two-particle correlation functions converges

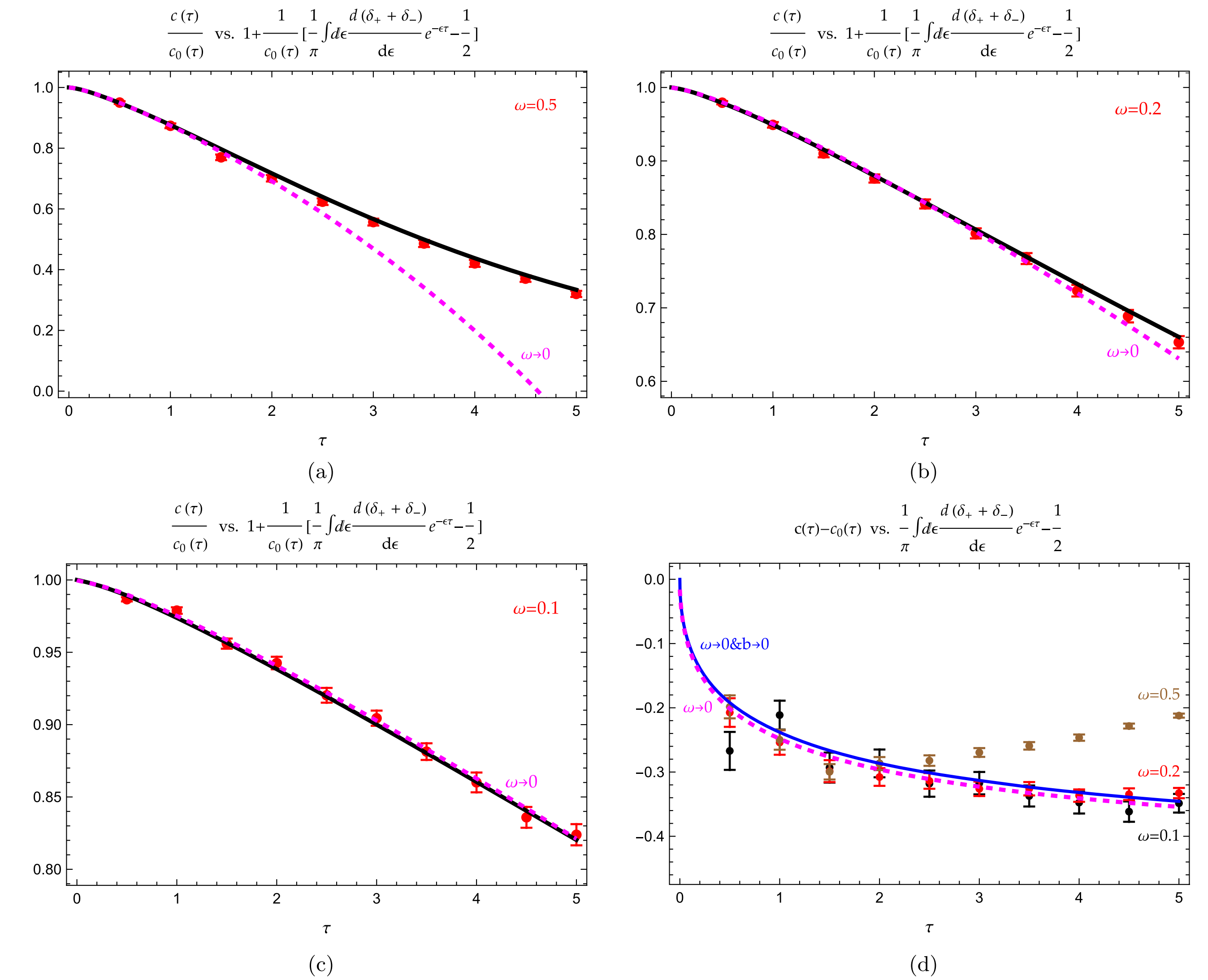


FIG. 5. Comparison of Monte Carlo data of $\frac{C(\tau)}{C_0(\tau)}$ vs infinite volume limit result for a spinless particle interacting with a square well potential in a harmonic oscillator trap for various ωs. In (a), (b), and (c), we plot Monte Carlo data (red error bars), exact solutions of $\frac{C(\tau)}{C_0(\tau)}$ by solving Hamiltonian matrix in Eq. (115) (solid black), and infinite volume limit result, $1+\frac{1}{C_0(\tau)}\left[\frac{1}{\pi}\int_0^\infty d\epsilon \frac{d(\delta_+ + \delta_-)}{d\epsilon} e^{-\epsilon\tau} - \frac{1}{2}\right]$ (dashed purple), for $\omega = 0.5$, 0.2, and 0.1, respectively. (d) Monte Carlo data of $C(\tau) - C_0(\tau)$ for various ωs: $\omega = 0.1$ (black), 0.2 (red), and 0.5 (brown), vs infinite volume limit result with a square well potential, $\frac{1}{\pi}\int_0^\infty d\epsilon \frac{d(\delta_+ + \delta_-)}{d\epsilon} e^{-\epsilon\tau} - \frac{1}{2}$ (dashed purple). The infinite volume limit result with a contact interaction potential, $V(r) = V_0\delta(r)$, is also plotted as a comparison in solid blue. The rest of parameters are taken as $V_0 = 1$, $\mu = 1$, and $b = 0.2$.

quickly to its infinite volume limit, which is expressed through an integral over the derivative of the phase shift weighted by an exponential factor. The fast convergent feature of proposed relation near small Euclidean times may have the potential to provide an alternative approach to traditional two-step Lüscher formula method. The ultimate goal is to develop an alternative method that can be a robust tool to extract phase shift from LQCD calculation especially in cases when the traditional two-step Lüscher formula method becomes less effective and determination of individual energy levels itself is already problematic, such as in nucleon-nucleon reactions. Much further work is required to accomplish this ultimate goal. The proposed approach will have to be extended to include relativistic dynamics, inelastic effect, etc. Monte Carlo simulation with field theory models are also demanded for the effectiveness and robustness test. We also remark that unlike Lüscher formula approach that relate energy levels to phase shift directly, our proposed approach requires the physics motivated modeling of phase shift and then fit to the LQCD data to fix model parameters. This resembles the procedure of determination of hadron-hadron scattering amplitudes from experimental data, see, e.g., Ref. [73]. The model of phase shift in principle can be further constrained by chiral perturbation theory, dispersion relation approach, Roy equation, etc., which can ultimately help to narrow down the parameter space in the model.

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APPENDIX A: QUANTIZATION CONDITION OF A TRAPPED TWO-PARTICLE SYSTEM IN $(1+1)$D

Some technical details of the derivation of quantization condition of trapped two-particle system in $(1+1)$D are given in this appendix. Let us consider two particles interacting with a contact interaction in a trap: the two particles could be either spinless particles or two fermions in spin singlet state. Hence only even parity state will be affected by contact interaction. The dynamics of relative motion of trapped two-particle systems are described by (1) Eq. (65) for a periodic box, wave function satisfies periodic boundary condition of wave function in Eq. (48); and (2) Eq. (73) for a harmonic oscillator trap.

The integral representation of dynamics of trapped systems are given by the Lippmann-Schwinger equation,

$$\psi_\epsilon^{(\mathrm{rel})}(r) = \int_{\mathrm{trap}} dr' G_0^{(\mathrm{trap})}(r, r'; \epsilon) V_0 \delta(r') \psi_\epsilon^{(\mathrm{rel})}(r'), \quad \text{(A1)}$$

where

$$\int_{\mathrm{trap}} dr' = \begin{cases} \int_{-\frac{L}{2}}^{\frac{L}{2}} dr', & \text{for a periodic box} \\ \int_{-\infty}^{\infty} dr', & \text{for a h.o. trap} \end{cases}. \quad \text{(A2)}$$

The $G_0^{(\mathrm{trap})}(r, r'; \epsilon)$ is Green's function of noninteracting particles in a trap: (1) for a periodic box, it satisfies differential equation,

$$\left[\epsilon + \frac{1}{2\mu}\frac{d^2}{dr^2}\right] G_0^{(\mathrm{trap})}(r, r'; \epsilon) = \sum_{n\in\mathbb{Z}} \delta(r - r' + nL), \quad \text{(A3)}$$

and periodic boundary condition,

$$G_0^{(\mathrm{trap})}(r + nL, r'; \epsilon) = G_0^{(\mathrm{trap})}(r, r'; \epsilon);$$

and (2) for a harmonic oscillator trap, it satisfies the following equation:

$$\left[\epsilon + \frac{1}{2\mu}\frac{d^2}{dr^2} - \frac{1}{2}\mu\omega^2 r^2\right] G_0^{(\mathrm{trap})}(r, r'; \epsilon) = \delta(r - r'). \quad \text{(A4)}$$

Hence the discrete energy spectra are determined by the quantization condition,

$$\frac{1}{V_0} = G_0^{(\mathrm{trap})}(0, 0; \epsilon). \quad \text{(A5)}$$

The analytic expression of $G_0^{(\mathrm{trap})}(r, r'; \epsilon)$ can be obtained for both periodic box and harmonic oscillator trap:

(1) for a periodic box, see, e.g., Refs. [13,20,26]

$$G_0^{(\mathrm{trap})}(r, r'; \epsilon) = \frac{1}{L}\sum_{n\in\mathbb{Z}}^{p=\frac{2\pi n}{L}} \frac{e^{ip(r-r')}}{\epsilon - \frac{p^2}{2\mu}} = -\frac{i\mu}{k}\left[e^{ik|r-r'|} + \frac{2\cos k(r-r')}{e^{-ikL} - 1}\right], \quad \text{(A6)}$$

where $k = \sqrt{2\mu\epsilon}$;

(2) for a harmonic oscillator trap, see, e.g., Ref. [74],

$$G_0^{(\mathrm{trap})}(r, r'; \epsilon) = -\frac{\Gamma(\frac{1}{4} - \frac{\epsilon}{2\omega})}{2\omega(\pi r r')^{\frac{1}{2}}} M_{\frac{\epsilon}{2\omega}, -\frac{1}{4}}(\mu\omega r_<^2) \times W_{\frac{\epsilon}{2\omega}, -\frac{1}{4}}(\mu\omega r_>^2), \quad \text{(A7)}$$

where M and W are Whittaker functions as defined in Ref. [75], and $r_<$ and $r_>$ represent the lesser and greater of (r, r'), respectively.

We thus find

$$G_0^{(\mathrm{trap})}(0,0;\epsilon) = \begin{cases} \frac{\mu}{k}\cot(\frac{kL}{2}), & \text{for a periodic box} \\ -\frac{\sqrt{\mu}}{2\sqrt{\omega}}\frac{\Gamma(\frac{1}{4} - \frac{\epsilon}{2\omega})}{\Gamma(\frac{3}{4} - \frac{\epsilon}{2\omega})}, & \text{for a h.o. trap} \end{cases}. \quad \text{(A8)}$$

The analytic expression of a scattering phase shift for a contact interaction is given by Eq. (67),

$$\frac{1}{V_0} = -\frac{\mu}{k}\cot\delta(\epsilon).$$

Hence the quantization conditions for (1) a periodic box and (2) a harmonic oscillator trap can be written in the form of a Lüscher formula [4] and a BERW formula [5],

$$\cot\delta(\epsilon) - \mathcal{M}(\epsilon) = 0, \quad \text{(A9)}$$

where

$$\mathcal{M}(\epsilon) = \begin{cases} -\cot\left(\sqrt{2\mu\epsilon}\frac{L}{2}\right), & \text{for a periodic box} \\ \frac{\sqrt{\mu}}{2\sqrt{\omega}}\frac{\Gamma(\frac{1}{4}-\frac{\epsilon}{2\omega})}{\Gamma(\frac{3}{4}-\frac{\epsilon}{2\omega})}, & \text{for a h.o. trap} \end{cases}. \tag{A10}$$

It is worth mentioning that the superlattice structure that has great interest in condensed matter physics can be constructed by placing finite number of short-range interaction potentials inside of traps. For an example, assuming potential of a simple superlattice structure having the form of

$$V(r) = \sum_{i=1}^{N} V_i \delta(r - a_i), \tag{A11}$$

where a_i is the location of an ith contact potential in the trap, the quantization condition that determine discrete energy spectra can be obtained from Lippmann-Schwinger equation:

$$\det\left[\delta_{i,j} - V_j G_0^{(\text{trap})}(a_i, a_j; \epsilon)\right] = 0. \tag{A12}$$

With some mathematical manipulation, we can easily show that the QC in Eq. (A12) is consistent with the result that is derived from the characteristic determinant approach in Refs. [76,77]:

$$\det[D_N] = 0,$$

where

$$(D_N)_{i,j} = \delta_{i,j} - V_j G_0^{(\text{trap})}(a_j, a_j; \epsilon)\sqrt{Z_{i,j}}, \tag{A13}$$

and

$$Z_{i,j} = Z_{j,i} = \frac{G_0^{(\text{trap})}(r_i, r_j; \epsilon) G_0^{(\text{trap})}(r_j, r_i; \epsilon)}{G_0^{(\text{trap})}(r_i, r_i; \epsilon) G_0^{(\text{trap})}(r_j, r_j; \epsilon)}. \tag{A14}$$

We remark that the determinant in Eq. (A12) is directly related to the full Green's function of the system. The full Green's function of the system provides the transmission coefficient and the density of states when opened systems are considered, and gives the bound spectrum if the system is closed (see Refs. [76,77] for more details). The poles of Green's function are the zeros of the determinant in Eq. (A12) for a closed system. The characteristic determinant approach is a convenient formalism to determine the energy spectrum electrons in a layered system or get sufficiently complete description of electron behavior in a random potential without finding electron eigenfunctions.

APPENDIX B: FRIEDEL's FORMULA AND KREIN's THEOREM IN $(1+1)$D SCATTERING THEORY

A brief review of Friedel's formula and Krein's theorem in $(1+1)$D scattering theory is provided in this section, and a detailed discussion can be found in Refs. [64–68]. The derivation can also be made in a rather more general way from formal scattering theory and S-matrix formulation approach, see, e.g., Refs. [69,78].

In Refs. [64,65], J. Friedel showed that the difference between the integrated density of states of the interacting particles system, $n_E(x)$, and free particles system, $n_E^{(0)}(x)$, is related to the scattering phaseshifts by

$$\int_{-\infty}^{\infty} dx[n_E(x) - n_E^{(0)}(x)] = \frac{1}{\pi}\frac{d}{dE}\text{Tr}[\delta(E)], \tag{B1}$$

where $\delta(E)$ stands for the diagonal matrix of scattering phaseshifts. The local density of states of a interacting system, $n_E(x)$, can be defined through the imaginary part of Green's function by

$$n_E(x) = -\frac{1}{\pi}\text{Im}[\langle x|\hat{G}(E + i0)|x\rangle], \tag{B2}$$

where

$$\hat{G}(E) = \frac{1}{E - \hat{H}}$$

refers to full Green's function operator of an interacting particles system, and $\hat{H}$ stands for the Hamiltonian operator of the interacting particles system. The local density of states of free particles system, $n_E^{(0)}(x)$, is defined in a similar way,

$$n_E^{(0)}(x) = -\frac{1}{\pi}\text{Im}[\langle x|\hat{G}_0(E + i0)|x\rangle], \tag{B3}$$

where

$$\hat{G}_0(E) = \frac{1}{E - \hat{H}_0}$$

denotes the free particle's Green's function operator. The relation in Eq. (B1) is usually referred as the Friedel formula.

The real part (principal part) of Green's function can be constructed through imaginary part by Cauchy's integral theorem,

$$\int_{-\infty}^{\infty} dx \langle x|\hat{G}(E) - \hat{G}_0(E)|x\rangle = \frac{1}{\pi}\left[\int_{-\infty}^{-E_L} + \int_0^{\infty}\right] d\epsilon \frac{\int_{-\infty}^{\infty} dx \mathrm{Im}\langle x|\hat{G}(E) - \hat{G}_0(E)|x\rangle}{\epsilon - E}, \tag{B4}$$

where we have assumed that Green's functions has a physical branch cut along the positive real axis in complex E plane: $E \in [0, \infty]$, and an unphysical branch cut siting along negative real axis: $E \in [-\infty, -E_L]$, where $-E_L$ represents the branch point of unphysical cut. Using Eq. (B1), we therefore find that integrated Green's function is related to the scattering phaseshifts by

$$\int_{-\infty}^{\infty} dx \langle x|\hat{G}(E) - \hat{G}_0(E)|x\rangle = -\frac{1}{\pi}\left[\int_{-\infty}^{-E_L} + \int_0^{\infty}\right] d\epsilon \frac{\mathrm{Tr}[\delta(\epsilon)]}{(\epsilon - E)^2}. \tag{B5}$$

J.S. Faulkner [68] later on recognized that the relation in Eq. (B5) is equivalent to Krein's theorem [66,67] in spectral theory, where $-\frac{1}{\pi}\mathrm{Tr}[\delta(\epsilon)]$ is exactly the Krein's spectral shift function.

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