Path Integral Treatment of Singular Problems and Bound States: Quantum Mechanics

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Abstract

A path-integral approach for the computation of quantum-mechanical propagators and energy Green's functions is presented. Its effectiveness is demonstrated through its application to singular interactions, with particular emphasis on the inverse square potential—possibly combined with a delta-function interaction. The emergence of these singular potentials as low-energy nonrelativistic limits of quantum field theory is highlighted. Not surprisingly, the analogue of ultraviolet regularization is required for the interpretation of these singular problems.

I. INTRODUCTION

It has been generally recognized that the treatment of singular problems in quantum mechanics is notoriously difficult and plagued with ambiguities [1]. A complete solution of a typical quantum-mechanical problem with a singular potential requires the analysis of the scattering and bound-state sectors supplemented by a prescription, which can be conveniently formulated in the field-theory language of regularization and renormalization. Such a prescription establishes the necessary connection between the physics of a particular system and the corresponding renormalization of an ill-defined problem. As this paper demonstrates, much work is still needed in formulating and interpreting singular problems in quantum physics, particularly within the path-integral framework.

It is also generally accepted that our current understanding of bound states in quantum field theory—including relativistic effects and radiative corrections—is still unsatisfactory [2, 3]. Conceptually, the source of this deficiency lies in the apparent contradiction between the usual perturbative framework of quantum field theory and the intrinsic nonperturbative nature of bound states, which manifest themselves as poles of the S-matrix and can only be generated by summing an infinite set of Feynman diagrams. Therefore, one is forced to face simultaneously a plethora of technical difficulties, including issues of regularization and renormalization, nonrelativistic reductions, model dependence, and stability and controllability of the approximation scheme. Following the seminal work of Bethe and Salpeter [4] many techniques and ideas have been developed, including numerical schemes, and have been applied to both QED and QCD with various degrees of success. More recently, the use of effective Lagrangians has advanced the field considerably [5], and extensions to other fields of medium- and high-energy physics are underway.

In this paper we begin a program centered on the use of path integrals for a systematic study of singular problems in quantum physics and of the connection between field theory and quantum mechanics *vis-à-vis* the description of bound states. One of the main purposes of this approach is to formulate a complementary point of view that may shed light on the difficult problems posed by bound states in quantum field theory. It is to be expected that a more thorough understanding of these questions would eventually have a substantial impact on the development of modern nuclear physics within the chiral Lagrangian approach [5], as well as on atomic and molecular physics [1]. Even though the use of path integrals to

study bound states is hardly new, it has mainly been implemented within the framework of quantum mechanics and, until recently, only for regular potentials [6, 7]. In this paper, as we take the first steps in formulating this program, we are confronted with the problem of describing singular potentials beyond the Coulomb problem. In particular, we will concentrate upon the path-integral treatment of the very important case of the inverse square potential, $1/r^2$, the first-one with integer powers beyond the Coulomb case.

The quantum-mechanical inverse square potential has been extensively dealt with before via the Schrödinger equation [8–11], and to a lesser extent with path integrals [12–16]. A recent proposal for a comprehensive treatment of this problem was advanced within the Schrödinger-equation approach, properly combined with regularization and renormalization concepts borrowed from quantum field theory. This was done first for the one-dimensional case with a real-space regulator [9]; later, it was generalized to a complete analysis of the D-dimensional case using different regularization schemes [10, 11]. The current relevance of this problem stands out not only from its field-theory treatment but also from its recent application to the interaction between an electron and polar molecule, which was shown to be a simple manifestation of a quantum anomaly [17].

The main goals of the present paper are:

(i) To introduce a general framework for the computation of bound states and other "nonperturbative" results within the path-integral approach to quantum physics (Sec. II).

(ii) To reformulate the problem of the inverse square potential and reproduce the results of Ref. [10] within the path-integral framework (Secs. IV–VI).

(iii) To generalize the inverse square potential by the inclusion of delta-function interactions, with miscellaneous applications (Sec. V).

(iv) To highlight the emergence of singular potentials within the effective-field theory program and to sketch possible generalizations in quantum field theory (Sec. VII).

The treatment of more singular potentials and the development of the full-fledged quantum-field-theory case is in progress and will be reported elsewhere.

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II. GENERAL FRAMEWORK

A. Quantum-Mechanical Propagator

Consider now a particle of mass M subject to an interaction potential $V(\mathbf{r}, t)$ in D-dimensions. Its physics is completely described by the quantum-mechanical propagator or transition amplitude

$$K_D(\mathbf{r}'', \mathbf{r}'; t'', t') = \left\langle \mathbf{r}'' \left| \hat{T} \exp\left[-\frac{i}{\hbar} \int_{t'}^{t''} \hat{H} dt \right] \right| \mathbf{r}' \right\rangle , \tag{1}$$

where $\hat{T}$ is the time-ordering operator and $\hat{H}$ the Hamiltonian. The propagator admits the usual representation

$$K_D(\mathbf{r}'', \mathbf{r}'; t'', t') = \int_{\mathbf{r}(t')=\mathbf{r}'}^{\mathbf{r}(t'')=\mathbf{r}''} \mathcal{D}\mathbf{r}(t) \exp\left\{ \frac{i}{\hbar} S\left[\mathbf{r}(t)\right] (\mathbf{r}'', \mathbf{r}'; t'', t') \right\} \tag{2}$$

as a path integral, in which $S\left[\mathbf{r}(t)\right](\mathbf{r}'', \mathbf{r}'; t'', t')$ is the classical action functional associated with "paths" $\mathbf{r}(t)$ that connect the end points $\mathbf{r}(t') = \mathbf{r}', \mathbf{r}(t'') = \mathbf{r}''$. In anticipation of the derivations of Sec. III, we have carefully defined all the relevant variables in the functional dependence of $S\left[\mathbf{r}(t)\right](\mathbf{r}'', \mathbf{r}'; t'', t')$; specifically, the action is (i) a functional of $\mathbf{r}(t)$ and (ii) a function of the end-point variables $(\mathbf{r}'', \mathbf{r}'; t'', t')$, for every chosen $\mathbf{r}(t)$.

Equation (2) is the primitive construct from which we will advance a general technique for the evaluation of the physics of singular potentials. Furthermore, we would like to explicitly show how to supplement this technique with regularization *à la* field theory for the derivation of the renormalized physics of the inverse square potential—by itself and also combined with a delta-function interaction.

A careful analysis shows that one must exercise proper caution when evaluating Eq. (2) in non-Cartesian coordinates. For example, when considering central potentials and transforming into hyperspherical coordinates in D dimensions, one may need to consider extra terms of order $\hbar^2$ in the action. These extra terms arise whenever nonlinear transformations are implemented, a fact that has been established in quantum mechanics [18] and quantum field theory [19]. However, these technical difficulties can be altogether circumvented by adopting a time-sliced expression in Cartesian coordinates as the starting point in Eq. (2) and transforming coordinates *before* taking the continuum limit. Therefore, we introduce a partition of the time $T = t'' - t'$ into N equal discrete time units,

$$\mathcal{P}^{(N)}\{t', t''\} : \{t_0 \equiv t', t_1, \ldots, t_{N-1}, t_N \equiv t''\} , \tag{3}$$

which yields a time lattice of $(N+1)$ equidistant points

$$t_j = t' + j\epsilon \quad \epsilon = \frac{t'' - t'}{N} \quad (j = 0, \ldots, N+1) \,, \tag{4}$$

with the end points fixed as in Eq. (3). This procedure should be followed by taking the limit $N \to \infty$ only after all other calculations are completed. Correspondingly, in Eq. (2), the action is replaced by its discrete counterpart

$$S^{(N)}[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}](\mathbf{r}'', \mathbf{r}'; t'', t') = \sum_{j=0}^{N-1} \left[\frac{M(\mathbf{r}_{j+1} - \mathbf{r}_j)^2}{2\epsilon} - \epsilon V(\mathbf{r}_j, t_j) \right] \,, \tag{5}$$

in which $\mathbf{r}_j = \mathbf{r}(t_j)$, while the end points are $\mathbf{r}_0 \equiv \mathbf{r}'$ and $\mathbf{r}_N \equiv \mathbf{r}''$. It should be noticed that the variable N has been isolated as a superscript in order to emphasize its distinct nature in the limit $S^{(N)}[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}](\mathbf{r}'', \mathbf{r}'; t'', t') \to S[\mathbf{r}(t)](\mathbf{r}'', \mathbf{r}'; t'', t')$, with the variables $\{\mathbf{r}_1, \ldots \mathbf{r}_{N-1}\}$ asymptotically generating a "path" $\mathbf{r}(t)$. Then, Eq. (2) can be interpreted as a shorthand for the time-sliced expression

$$K_D(\mathbf{r}'', \mathbf{r}'; t'', t') = \lim_{N \to \infty} \int_{\mathbf{r}(t')=\mathbf{r}'}^{\mathbf{r}(t'')=\mathbf{r}''} \mathcal{D}^{(N)}\mathbf{r}(t) \exp\left\{ \frac{i}{\hbar} S^{(N)}[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}](\mathbf{r}'', \mathbf{r}'; t'', t') \right\} \,, \tag{6}$$

where the integration and measure symbols stand for the formal $(N-1)$-fold integral operation

$$\int_{\mathbf{r}(t')=\mathbf{r}'}^{\mathbf{r}(t'')=\mathbf{r}''} \mathcal{D}^{(N)}\mathbf{r}(t) \equiv [\mathcal{C}(M, \epsilon, \hbar, D)]^N \left[\prod_{k=1}^{N-1} \int_{\mathbb{R}^D} d^D \mathbf{r}_k \right] \,, \tag{7}$$

with

$$\mathcal{C}(M, \epsilon, \hbar, D) = \left(\frac{M}{2\pi i \epsilon \hbar} \right)^{D/2} \,. \tag{8}$$

As is well known, the propagator $K_D(\mathbf{r}'', \mathbf{r}'; t'', t')$ solves the initial-value problem for the Schrödinger equation, permitting the computation of the wave function $\Psi(\mathbf{r}, t)$ at any time t, given a particular-time value $\Psi(\mathbf{r}, t_0)$. A related quantity is the retarded (causal) Green's function $G_D(\mathbf{r}'', \mathbf{r}'; t'', t')$, which solves the Schrödinger equation with an additional arbitrary inhomogeneous term, and which is related to the propagator by

$$G_D(\mathbf{r}'', \mathbf{r}'; t'', t') = \theta(t'' - t') K_D(\mathbf{r}'', \mathbf{r}'; t'', t') \,, \tag{9}$$

where $\theta(T)$ stands for the Heaviside function.

In this paper we will consider time-independent singular potentials, with special emphasis on the inverse square potential and the delta-function interaction. These particular cases are included in the class of time-independent Hamiltonians, for which the lattice action

$$S^{(N)}[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}](\mathbf{r}'', \mathbf{r}'; t'', t') \equiv S^{(N)}[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}](\mathbf{r}'', \mathbf{r}'; t'' - t') \,, \tag{10}$$

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as well as its continuum limit

$$S\left[\mathbf{r}(t)\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right) \equiv S\left[\mathbf{r}(t)\right]\left(\mathbf{r}'', \mathbf{r}'; t'' - t'\right), \tag{11}$$

and the propagator

$$K_D(\mathbf{r}'', \mathbf{r}'; t'', t') \equiv K_D(\mathbf{r}'', \mathbf{r}'; t'' - t') \tag{12}$$

are functions of the end-point times t' and t'' only through the difference $T = t'' - t'$. Under this assumption, it is also possible to specialize to "paths" connecting the end points $\mathbf{r}(0) = \mathbf{r}', \mathbf{r}(T) = \mathbf{r}''$. Then, the Fourier transform of $G_D(\mathbf{r}'', \mathbf{r}'; T)$ with respect to T defines the corresponding energy Green's function

$$
\begin{aligned}
G_D(\mathbf{r}'', \mathbf{r}'; E) &= \frac{1}{i\hbar} \int_{-\infty}^{\infty} dT\, e^{iET/\hbar} G_D(\mathbf{r}'', \mathbf{r}'; T) \\
&= \frac{1}{i\hbar} \int_{0}^{\infty} dT\, e^{iET/\hbar} K_D(\mathbf{r}'', \mathbf{r}'; T) \\
&= \frac{1}{i\hbar} \int_{0}^{\infty} dT \int_{\mathbf{r}(0)=\mathbf{r}'}^{\mathbf{r}(T)=\mathbf{r}''} \mathcal{D}\mathbf{r}(t) \exp\left(\frac{i}{\hbar}\left\{S\left[\mathbf{r}(t)\right]\left(\mathbf{r}'', \mathbf{r}'; T\right) + ET\right\}\right).
\end{aligned}
$$
(13)
(14)

The energy Green's function is a convenient tool for spectral analyses because it satisfies the operator relation

$$G_D(\mathbf{r}'', \mathbf{r}'; E) = \left\langle \mathbf{r}'' \left| \left(E - \hat{H} + i\epsilon\right)^{-1} \right| \mathbf{r}' \right\rangle, \tag{15}$$

where $i\epsilon$ is a small positive imaginary part—this follows by combining Eqs. (1) and (13). In particular, it admits a spectral representation,

$$G_D(\mathbf{r}'', \mathbf{r}'; E) = \sum_n \frac{\psi_n(\mathbf{r}'')\,\psi_n^*(\mathbf{r}')}{E - E_n + i\epsilon} + \int d\alpha\, \frac{\psi_\alpha(\mathbf{r}'')\,\psi_\alpha^*(\mathbf{r}')}{E - E_\alpha + i\epsilon}, \tag{16}$$

which identifies the bound states as poles and the scattering states as branch cuts, as well as the corresponding stationary wave functions [6]. For example, for a nondegenerate bound state of energy E_n, the wave function $\psi_n(\mathbf{r}) = |\psi_n(\mathbf{r})|e^{i\delta_n(\mathbf{r})}$ can be uniquely extracted, up to an arbitrary global phase factor, from

$$|\psi_n(\mathbf{r})| = |\text{Res}\left\{G(\mathbf{r}, \mathbf{r}; E_n)\right\}|^{1/2} \tag{17}$$

and

$$\delta_n(\mathbf{r}) = -i \ln \left\{ \frac{\text{Res}\left\{G(\mathbf{r}, \mathbf{r}_0; E_n)\right\}}{\left[\text{Res}\left\{G(\mathbf{r}, \mathbf{r}; E_n)\right\} \text{Res}\left\{G(\mathbf{r}_0, \mathbf{r}_0; E_n)\right\}\right]^{1/2}} \right\}, \tag{18}$$

where $\mathbf{r}_0$ is a convenient reference point and $\mathrm{Res}\{f(z_0)\}$ represents the residue of the function $f(z)$ at the pole $z = z_0$.

In what follows our arguments and derivations will be based on Eqs. (6) and (14), as well as on their counterparts in hyperspherical coordinates, which we will consider next.

B. Central Interactions

For the all-important class of central potentials, Eq. (6) can be conveniently rewritten in hyperspherical polar coordinates [10, 11, 20]. This can be accomplished by separation of variables, a procedure that can be systematically implemented by repeated use of the addition formula [21] $e^{iz\cos\psi} = (iz/2)^{-\nu}\Gamma(\nu)\sum_{l=0}^{\infty}(l+\nu)I_{l+\nu}(iz)C_l^{(\nu)}(\cos\psi)$, where $I_p(x)$ is the modified Bessel function of the first kind and order p, $C_l^{(\nu)}(x)$ is a Gegenbauer polynomial, and $\nu = D/2 - 1$ is a related dimensionality parameter. In turn, the Gegenbauer polynomials can be resolved into hyperspherical harmonics $Y_{lm}(\mathbf{\Omega})$, labeled with the D-dimensional angular momentum quantum numbers l and m, where the latter has a multiplicity $d_l = (2l + D - 2)(l + D - 3)!/l!(D-2)!$ [20]. As a result, the propagator admits the partial-wave expansions

$$
\begin{aligned}
K_D(\mathbf{r}'', \mathbf{r}'; T) &= \frac{\Gamma(\nu)}{2\pi^{D/2}}\,(r''r')^{-(D-1)/2}\sum_{l=0}^{\infty}(l+\nu)\,C_l^{(\nu)}(\cos\psi_{\mathbf{\Omega}'',\mathbf{\Omega}'})\,K_{l+\nu}(r'', r'; T) \\
&= (r''r')^{-(D-1)/2}\sum_{l=0}^{\infty}\sum_{m=1}^{d_l}Y_{lm}(\mathbf{\Omega}'')Y_{lm}^{*}(\mathbf{\Omega}')\,K_{l+\nu}(r'', r'; T)\,,
\end{aligned}
\tag{19}
$$

where $\cos\psi_{\mathbf{\Omega}'',\mathbf{\Omega}'} = \hat{\mathbf{r}}''\cdot\hat{\mathbf{r}}'$ and the radial prefactors are conveniently written so that, for each angular momentum channel l, the radial propagator $K_{l+\nu}(r'', r'; T)$ satisfies the composition property

$$
K_{l+\nu}(r'', r'; t'' - t') = \int_0^{\infty} dr\, K_{l+\nu}(r'', r; t'' - t)K_{l+\nu}(r, r'; t - t')\,.
\tag{20}
$$

Moreover, the radial propagator in Eq. (19) can be explicitly evaluated by means of the path-integral expression

$$
\begin{aligned}
K_{l+\nu}(r'', r'; T) = \lim_{N\to\infty}\left(\frac{M}{2\pi i\epsilon\hbar}\right)^{N/2}\prod_{k=1}^{N-1}\left[\int_0^{\infty}dr_k\right]\mu_{l+\nu}^{(N)}[r^2] \\
\times\,\exp\left\{\frac{i}{\hbar}R^{(N)}[r_1,\dots r_{N-1}](r'', r'; T)\right\}\,,
\end{aligned}
\tag{21}
$$

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where the radial action is

$$R^{(N)}[r_1, \ldots r_{N-1}](r'', r'; T) = \sum_{j=0}^{N-1} \left[\frac{M(r_{j+1} - r_j)^2}{2\epsilon} - \epsilon V(r_j) \right] . \tag{22}$$

In Eq. (21) a radial functional weight

$$\mu_{l+\nu}^{(N)}[r^2] = \prod_{j=0}^{N-1} \left[\sqrt{2\pi z_j} e^{-z_j} I_{l+\nu}(z_j) \right] \tag{23}$$

has been properly defined with the radial variables appearing through the characteristic dimensionless ratio

$$z_j = \frac{M r_j r_{j+1}}{i\epsilon\hbar} . \tag{24}$$

As a consequence, the radial path integral, supplemented by the condition $r(t) \geq 0$, can be given a formal continuum representation

$$K_{l+\nu}(r'', r'; T) = \int_{r(0)=r'}^{r(T)=r''} \mathcal{D}r(t) \, \mu_{l+\nu}[r^2] \exp\left(\frac{i}{\hbar} \int_0^T dt \left\{ \frac{M}{2} \left[\dot{r}(t) \right]^2 - V(r(t)) \right\} \right) \tag{25}$$

in terms of the usual one-dimensional path-integral pseudomeasure $\mathcal{D}r(t)$. However, our subsequent analysis will be based on the time-sliced Eq. (21), which has been called a Besselian path integral [16] because of the appearance of modified Bessel functions in the pseudomeasure (23). A similar approach can be applied to the energy Green's function $G_D(\mathbf{r}'', \mathbf{r}'; E)$, which through a partial-wave expansion of the form (19) defines a radial counterpart

$$G_{l+\nu}(r'', r'; E) = \frac{1}{i\hbar} \int_0^\infty dT e^{iET/\hbar} K_{l+\nu}(r'', r'; T) . \tag{26}$$

It should be noticed that Eqs. (21)–(26) explicitly exhibit a property that may be called interdimensional dependence [22]: D and l appear in the combination $l + \nu$.

It is well known that the path-integral expression (21) for the free-particle radial propagator can be computed analytically and exactly (even before taking the continuum limit, $N \to \infty$), with the familiar result [13]

$$K_{l+\nu}^{(0)}(r'', r'; T) = \frac{M}{i\hbar T} \sqrt{r'r''} \exp\left[\frac{iM}{2\hbar T} \left(r'^2 + r''^2 \right) \right] I_{l+\nu}\left(\frac{Mr'r''}{i\hbar T} \right) ; \tag{27}$$

this is accomplished through the use of Bessel-function identities and recursion relations [23]. In addition, the Fourier transform (26) of $K_{l+\nu}^{(0)}(r'', r'; T)$ [24] provides a closed analytical expression for the free-particle radial energy Green's function

$$G_{l+\nu}^{(0)}(r'', r'; E) = -\frac{2M}{\hbar^2} \sqrt{r'r''} I_{l+\nu}(\kappa r_<) K_{l+\nu}(\kappa r_>) , \tag{28}$$

in which the energy variable appears in the combination

$$\kappa = \frac{\sqrt{-2ME}}{\hbar} .$$ (29)

As usual, in Eq. (28), $r_<$ ($r_>$) is the smaller (larger) of r' and r'', while $I_p(x)$ and $K_p(x)$ are the modified Bessel functions of the first kind and second kind (and order p) respectively.

Explicit evaluation of Eq. (21) beyond the free-particle case has been accomplished only in a few special cases, including the radial harmonic oscillator [16], using miscellaneous limiting procedures in the limit $N \to \infty$. For the case of more general potentials, we will next describe a technique that permits the summation of perturbation-theory contributions to all orders.

III. INFINITE SUMMATION OF PERTURBATION THEORY

In this section we introduce a general technique that consists of a perturbation expansion followed by its summation to all orders—this is essentially the "perturbation approach" pioneered in Refs. [15, 25]. The objective of this combined procedure is to extract "nonperturbative" results, including the emergence of bound states (whenever appropriate), from a manifestly perturbative scheme. This is only possible by summing the perturbative series to all orders. We generalize the results of Refs. [15, 25] in a number of ways: (i) we present the theory in any number of dimensions, for the full-fledged propagator and for the Green's function; (ii) we develop it within the time-sliced formulation of path integrals, with emphasis upon possible subtleties involved in nonlinear coordinate changes; and (iii) we explicitly show that the expansion for radial path integrals does not require any additional modifications, provided that the Besselian pseudomeasure (23) be used at every order. At the very least, this technique will play a crucial role in providing a complete and satisfactory derivation of the renormalized physics of the inverse square potential and delta-function interactions.

A. Perturbation Theory

This procedure is based on the standard resolution of the action in the form

$$
\begin{aligned}
S\left[\mathbf{r}(t)\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right) &= S^{(0)}\left[\mathbf{r}(t)\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right) + \tilde{S}\left[\mathbf{r}(t)\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right) \\
&= S^{(0)}\left[\mathbf{r}(t)\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right) - \int_{t'}^{t''} dt\, V(\mathbf{r}(t), t) ,
\end{aligned}
\tag{30}
$$

where $S^{(0)}\left[\mathbf{r}(t)\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right)$ is the action for a problem whose propagator is already known (for example, the free-particle action) while $\tilde{S}\left[\mathbf{r}(t)\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right)$ provides the additional interactions $V(\mathbf{r}, t)$ in $S\left[\mathbf{r}(t)\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right)$.

Even though this beginning step (30) looks like standard perturbation theory, it is in fact intended as an exact rearrangement based on infinite summations performed to all orders. This resolution can be applied to any path-integral expression: to Eq. (6), for the full-fledged D-dimensional problem; and to Eq. (21), for the radial propagator. Just as before, the time-lattice versions guarantee that all subtleties are properly accounted for in this formulation. Thus, we will start with a lattice action described by the generic Eqs. (5)–(8), as defined by the associated partition (3), i.e.,

$$
\begin{aligned}
S^{(N)}\left[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right) &= S^{(0;N)}\left[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right) + \tilde{S}^{(N)}\left[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right) \\
&= S^{(0;N)}\left[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right) - \epsilon \sum_{j=0}^{N-1} V(\mathbf{r}_j, t_j)
\end{aligned}
\tag{31}
$$

in lieu of Eq. (30), where $S^{(0;N)}$ stands for the corresponding lattice unperturbed action. In each one of these path integrals, the exponential $e^{i\tilde{S}^{(N)}/\hbar}$ is to be expanded to all orders,

$$
\begin{aligned}
&\exp\left\{\frac{i}{\hbar}\tilde{S}^{(N)}\left[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right)\right\} \\
&= \sum_{n=0}^{\infty} \frac{\epsilon^n}{n!}\left[\sum_{j_n=0}^{N-1} \cdots \sum_{j_1=0}^{N-1} \frac{V(\mathbf{r}_{j_n}, t_{j_n})}{i\hbar} \cdots \frac{V(\mathbf{r}_{j_1}, t_{j_1})}{i\hbar}\right] \\
&= \sum_{n=0}^{\infty} \epsilon^n\left[\sum_{j_1 < j_2 < \cdots < j_n = 0}^{N-1} \frac{V(\mathbf{r}_{j_n}, t_{j_n})}{i\hbar} \cdots \frac{V(\mathbf{r}_{j_1}, t_{j_1})}{i\hbar}\right]\left[1 + O\left(\frac{1}{N}\right)\right] ,
\end{aligned}
\tag{32}
$$

where corrections of order $O(1/N)$ are associated with the terms with repeated indices. In order to simplify the notation, while at the same time preventing ambiguities, let us define

$$
\begin{aligned}
t_{(0)} &\equiv t_0 = t' & t_{(n+1)} &\equiv t_N = t'' \\
t_{(\alpha)} &\equiv t_{j_\alpha} & \mathbf{r}_{(\alpha)} &\equiv \mathbf{r}_{j_\alpha} & (\alpha = 1, \ldots, n) .
\end{aligned}
\tag{33}
$$

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Then, *at each order of perturbation theory*, Eq. (32) defines a time ordering with which we can associate the partition

$$\mathcal{P}^{(n+1)}\left\{t', t''\right\} : \left\{t_{(0)} \equiv t', t_{(1)}, t_{(2)}, \ldots, t_{(n)}, t_{(n+1)} \equiv t''\right\} \tag{34}$$

leading to a resolution of the unperturbed action

$$
\begin{aligned}
S^{(0;N)}\left[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right) &\equiv S^{(0;N)}\left[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}\right]\left(\mathbf{r}'', \mathbf{r}'; t'', t'\right) \\
&= \sum_{\alpha=0}^{n} S^{(0;N)}\left[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}\right]\left(\mathbf{r}_{(\alpha+1)}, \mathbf{r}_{(\alpha)}; t_{(\alpha+1)}, t_{(\alpha)}\right) . \tag{35}
\end{aligned}
$$

In Eq. (35) the whole interval $T = t'' - t'$ has been divided into $n+1$ subintervals $T_{(\alpha)} = t_{(\alpha+1)} - t_{(\alpha)}$, by introducing the points $t_{(\alpha)}$ with $\alpha = 0, \ldots, n+1$, at each order n in perturbation theory. Correspondingly, the D-dimensional propagator becomes

$$K_D(\mathbf{r}'', \mathbf{r}'; t'', t') = \sum_{n=0}^{\infty} K_D^{(n)}(\mathbf{r}'', \mathbf{r}'; t'', t') , \tag{36}$$

in which the n-th order contribution is

$$
\begin{aligned}
K_D^{(n)}(\mathbf{r}'', \mathbf{r}'; t'', t') &= \lim_{N \to \infty} \int_{\mathbf{r}(t')=\mathbf{r}'}^{\mathbf{r}(t'')=\mathbf{r}''} \mathcal{D}^{(N)}\mathbf{r}(t) \\
&\times \epsilon^n \left[\sum_{j_1 < j_2 < \cdots < j_n = 0}^{N-1} \frac{V(\mathbf{r}_{j_n}, t_{j_n})}{i\hbar} \cdots \frac{V(\mathbf{r}_{j_1}, t_{j_1})}{i\hbar}\right] \left[1 + O\left(\frac{1}{N}\right)\right]\bigg|_{\left\{t_{j_\alpha} \equiv t_{(\alpha)}; \mathbf{r}_{j_\alpha} \equiv \mathbf{r}_{(\alpha)}\right\}} \\
&\times \prod_{\beta=0}^{n} \left[\exp\left\{\frac{i}{\hbar} S^{(0;N)}\left[\mathbf{r}_1, \ldots \mathbf{r}_{N-1}\right]\left(\mathbf{r}_{(\beta+1)}, \mathbf{r}_{(\beta)}; t_{(\beta+1)}, t_{(\beta)}\right)\right\}\right] , \tag{37}
\end{aligned}
$$

with the time-sliced measure displayed in Eqs. (7) and (8). Finally, before taking the limit $N \to \infty$ in Eq. (37), it is suitable to assume that $N \gg n$, followed by a rearrangement of the time lattice according to the following scheme:

(i) The whole time interval $T = t'' - t'$ is divided into $n+1$ subintervals just as in Eq. (35).

(ii) Each subinterval $[t_{(\alpha)}, t_{(\alpha+1)}]$ is partitioned in the usual way into N_α parts, just as in Eq. (3), i.e.,

$$\mathcal{P}^{(N_\alpha)}\left\{t_{(\alpha)}, t_{(\alpha+1)}\right\} : \left\{t_{\alpha, j_0} \equiv t_{(\alpha)}, t_{\alpha, j_1}, \ldots, t_{\alpha, j_{N_\alpha-1}}, t_{\alpha, j_{N_\alpha}} \equiv t_{(\alpha+1)}\right\} . \tag{38}$$

(iii) Therefore, the whole interval consists of the following sub-partitions

$$\mathcal{P}^{(N)}\left\{t', t''\right\} = \left\{\mathcal{P}^{(N_0)}\left\{t', t_1\right\}; \mathcal{P}^{(N_1)}\left\{t_1, t_2\right\}; \ldots; \mathcal{P}^{(N_n)}\left\{t_n, t''\right\}\right\} , \tag{39}$$

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where the notational redefinition implied in Eq. (38) makes the parentheses surrounding the subscript α redundant. Thus, the omission of these parentheses amounts to the replacements

$$t_{(\alpha)} \hookrightarrow t_\alpha \tag{40}$$

$$\mathbf{r}_{(\alpha)} \hookrightarrow \mathbf{r}_\alpha , \tag{41}$$

which will be assumed in our subsequent discussion. With the partition defined by Eqs. (38) and (39), a partial measure $\mathcal{D}^{(N_\alpha)}\mathbf{r}(t)$ is defined just as in Eq. (7), with the result

$$\int_{\mathbf{r}(t')=\mathbf{r}'}^{\mathbf{r}(t'')=\mathbf{r}''} \mathcal{D}^{(N)}\mathbf{r}(t) = \prod_{\alpha=1}^{n}\left[\int d^D\mathbf{r}_\alpha\right] \prod_{\beta=0}^{n}\left[\int_{\mathbf{r}(t_\beta)=\mathbf{r}_\beta}^{\mathbf{r}(t_{\beta+1})=\mathbf{r}_{\beta+1}} \mathcal{D}^{(N_\beta)}\mathbf{r}(t)\right] , \tag{42}$$

where the first set of integration factors represents the contribution from the end points of each subinterval—conveniently singled out in order to avoid overcounting. Remarkably, in Eq. (42), the factors $\mathcal{C}(M,\epsilon,\hbar,D)$ [from Eqs. (7) and (8)] naturally redistribute in such a way that each subinterval inherits the proper measure.

Finally, in the limit $N \to \infty$,

$$\epsilon^n\left[\sum_{j_1<j_2<\cdots<j_n=0}^{N-1} \frac{V(\mathbf{r}_{j_n},t_{j_n})}{i\hbar}\cdots\frac{V(\mathbf{r}_{j_1},t_{j_1})}{i\hbar}\right]\left[1+O\left(\frac{1}{N}\right)\right]$$

$$\overset{(N\to\infty)}{\longrightarrow} \int_{t'}^{t''}dt_n\int_{t'}^{t_n}dt_{n-1}\ldots\int_{t'}^{t_3}dt_2\int_{t'}^{t_2}dt_1 \frac{V(\mathbf{r}_n,t_n)}{i\hbar}\cdots\frac{V(\mathbf{r}_1,t_1)}{i\hbar} . \tag{43}$$

Then, as a result of the integration measure (42), Eq. (37) takes the form

$$K_D^{(n)}(\mathbf{r}'',\mathbf{r}';t'',t') = \int_{t'}^{t''}dt_n\int_{t'}^{t_n}dt_{n-1}\ldots\int_{t'}^{t_2}dt_1$$

$$\times \prod_{\alpha=1}^{n}\left[\int d^D\mathbf{r}_\alpha\frac{V(\mathbf{r}_\alpha,t_\alpha)}{i\hbar}\right]\prod_{\beta=0}^{n}\left[K_D^{(0)}(\mathbf{r}_{\beta+1},\mathbf{r}_\beta;t_{\beta+1},t_\beta)\right] , \tag{44}$$

where the contributions from $S^{(0)}\left[\mathbf{r}(t)\right](\mathbf{r}_{\beta+1},\mathbf{r}_\beta;t_{\beta+1},t_\beta)$ have been converted into the propagators $K_D^{(0)}(\mathbf{r}_{\beta+1},\mathbf{r}_\beta;T_\beta)$, as $N \to \infty$. For the particular case of time-independent Hamiltonians, Eq. (44) can be recast into the alternative expressions

$$K_D^{(n)}(\mathbf{r}'',\mathbf{r}';T) = \prod_{\alpha=1}^{n}\left[\int d^D\mathbf{r}_\alpha\frac{V(\mathbf{r}_\alpha)}{i\hbar}\right]$$

$$\times \int_{t'}^{t''}dt_n\int_{t'}^{t_n}dt_{n-1}\ldots\int_{t'}^{t_2}dt_1\prod_{\beta=0}^{n}\left[K_D^{(0)}(\mathbf{r}_{\beta+1},\mathbf{r}_\beta;t_{\beta+1}-t_\beta)\right] \tag{45}$$

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and

$$K_D^{(n)}(\mathbf{r}'', \mathbf{r}'; T) = \prod_{\alpha=1}^{n} \left[\int d^D \mathbf{r}_\alpha \frac{V(\mathbf{r}_\alpha)}{i\hbar} \right] \prod_{\beta=0}^{n} \left[\int_0^\infty dT_\beta K_D^{(0)}(\mathbf{r}_{\beta+1}, \mathbf{r}_\beta; T_\beta) \right] \delta \left(T - \sum_{\gamma=0}^{n} T_\gamma \right) ; \tag{46}$$

correspondingly, from Eq. (46), the Fourier transform defining the energy Green's function yields the result

$$G_D(\mathbf{r}'', \mathbf{r}'; E) = \sum_{n=0}^{\infty} G_D^{(n)}(\mathbf{r}'', \mathbf{r}'; E) , \tag{47}$$

with an n-th order contribution

$$G_D^{(n)}(\mathbf{r}'', \mathbf{r}'; E) = \prod_{\alpha=1}^{n} \left[\int_0^\infty d^D \mathbf{r}_\alpha V(\mathbf{r}_\alpha) \right] \prod_{\beta=0}^{n} \left[G_D^{(0)}(\mathbf{r}_{\beta+1}, \mathbf{r}_\beta; E) \right] . \tag{48}$$

Direct comparison of Eqs. (45) and (48) shows that the former displays characteristic extra integrations with respect to time; these arise when separating the end points of each subinterval in the time-sliced expressions. Moreover, the perturbation expansions based on Eqs. (36)–(48) admit the usual diagrammatic representations.

B. Central Potentials

For the case of central potentials, the same procedure can be directly applied to the radial path integrals, with their respective Besselian pseudomeasures (23) at each order. Alternatively, Eqs. (36)–(48) could be resolved in hyperspherical coordinates term by term—as in the derivation leading to Eq. (19). Either derivation yields the exact infinite summation

$$K_{l+\nu}(r'', r'; T) = \sum_{n=0}^{\infty} K_{l+\nu}^{(n)}(r'', r'; T) , \tag{49}$$

for the propagator, where

$$\begin{aligned} K_{l+\nu}^{(n)}(r'', r'; T) &= \prod_{\alpha=1}^{n} \left[\int_0^\infty dr_\alpha \frac{V(r_\alpha)}{i\hbar} \right] \\ &\times \int_{t'}^{t''} dt_n \int_{t'}^{t_n} dt_{n-1} \ldots \int_{t'}^{t_2} dt_1 \prod_{\beta=0}^{n} \left[K_{l+\nu}^{(0)}(r_{\beta+1}, r_\beta; t_{\beta+1} - t_\beta) \right] , \end{aligned} \tag{50}$$

Correspondingly, the energy Green's function associated with Eqs. (49) and (50) is

$$G_{l+\nu}(r'', r'; E) = \sum_{n=0}^{\infty} G_{l+\nu}^{(n)}(r'', r'; E) , \tag{51}$$

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where

$$G_{l+\nu}^{(n)}(r'', r'; E) = \prod_{\alpha=1}^{n} \left[\int_0^\infty dr_\alpha V(r_\alpha) \right] \prod_{\beta=0}^{n} \left[G_{l+\nu}^{(0)}(r_{\beta+1}, r_\beta; E) \right] . \tag{52}$$

Finally, in subsequent applications it will prove convenient to introduce the reduced functions $\mathcal{V}(r)$ and $\mathcal{G}_{l+\nu}^{(n)}(r'', r'; E)$, implicitly defined from

$$V(r) = -\frac{\hbar^2}{2M} \lambda \mathcal{V}(r) \tag{53}$$

and

$$G_{l+\nu}^{(n)}(r'', r'; E) = -\frac{2M}{\hbar^2} |\mathcal{V}(r'')\mathcal{V}(r')|^{-1/2} \mathcal{G}_{l+\nu}^{(n)}(r'', r'; E) , \tag{54}$$

as well as the sign symbol $\epsilon_{r_\alpha} = \mathrm{sgn}\,(r_\alpha)$. These substitutions lead to the reduced perturbation expansion

$$\mathcal{G}_{l+\nu}(r'', r'; E) = \sum_{n=0}^{\infty} \mathcal{G}_{l+\nu}^{(n)}(r'', r'; E) , \tag{55}$$

with

$$\mathcal{G}_{l+\nu}^{(n)}(r'', r'; E) = \lambda^n \prod_{\alpha=1}^{n} \left[\int_0^\infty dr_\alpha \, \epsilon_{r_\alpha} \right] \prod_{\beta=0}^{n} \left[\mathcal{G}_{l+\nu}^{(0)}(r_{\beta+1}, r_\beta; E) \right] . \tag{56}$$

Notice that, even for $n = 0$ in Eq. (54), the "unperturbed" function $\mathcal{G}_{l+\nu}^{(0)}(r'', r'; E)$ already includes information about the perturbation $\mathcal{V}(r)$.

C. Integral Representations

The perturbation-theory framework of the previous subsection can be further extended when $\mathcal{V}(r)$ is a monotonic function. This is precisely the case for the class of power-law interactions—including the inverse square potential. When this condition is satisfied, the sign symbols ϵ_{r_α} in Eq. (56) can be omitted altogether. As a result, the perturbation expansion of Eqs. (55) and (56) reduces to the evaluation of

$$\begin{aligned} \mathcal{G}_{l+\nu}^{(n)}(r'', r'; E) &= \lambda^n \int_0^\infty dr_n \ldots \int_0^\infty dr_1 \\ &\times \mathcal{G}_{l+\nu}^{(0)}(r'', r_n; E)\mathcal{G}_{l+\nu}^{(0)}(r_n, r_{n-1}; E) \ldots \mathcal{G}_{l+\nu}^{(0)}(r_2, r_1; E)\mathcal{G}_{l+\nu}^{(0)}(r_1, r'; E) . \end{aligned} \tag{57}$$

The formal structure of Eq. (57) can be interpreted to be of the operator form

$$\hat{\mathcal{G}}_{l+\nu}^{(n)}(E) = \lambda^n \left[\hat{\mathcal{G}}_{l+\nu}^{(0)}(E) \right]^{n+1} , \tag{58}$$

according to the prescriptions presented in the Appendix, with operator products evaluated in real space. This observation leads to a reconstruction of the operator $\hat{\mathcal{G}}_{l+\nu}^{(n)}(E)$ in terms of the eigenvalues of $\hat{\mathcal{G}}_{l+\nu}^{(0)}(E)$, as the following argument shows.

First, suppose that the eigenvalues and eigenvectors of the self-adjoint operator $\hat{\mathcal{G}}_{l+\nu}^{(0)}(E)$ are labeled with an index z and known to be $\eta_{l+\nu}(z;\kappa)$ and $\Psi_{z,l+\nu}(\kappa)$ respectively, where κ is given by Eq. (29). In symbolic notation,

$$\hat{\mathcal{G}}_{l+\nu}^{(0)}(E)\,\Psi_{z,l+\nu}(\kappa) = \eta_{l+\nu}(z;\kappa)\,\Psi_{z,l+\nu}(\kappa)\,, \tag{59}$$

which stands for the integral relation

$$\int_0^\infty dr'\,\mathcal{G}_{l+\nu}^{(0)}(r,r';E)\Psi_{z,l+\nu}(r';\kappa) = \eta_{l+\nu}(z;\kappa)\Psi_{z,l+\nu}(r;\kappa)\,. \tag{60}$$

Second, in operator symbolic notation, Eq. (58) is equivalent to the eigenvalue equation

$$\hat{\mathcal{G}}_{l+\nu}^{(n)}(E)\,\Psi_{z,l+\nu}(\kappa) = \lambda^n\,[\eta_{l+\nu}(z;\kappa)]^{n+1}\,\Psi_{z,l+\nu}(\kappa)\,. \tag{61}$$

Third, the corresponding eigenvalue equation for the radial Green's function operator $\hat{\mathcal{G}}_{l+\nu}(E)$ can be obtained by geometrically *summing the entire perturbation series*,

$$\hat{\mathcal{G}}_{l+\nu}(E)\,\Psi_{z,l+\nu}(\kappa) = \frac{1}{[\eta_{l+\nu}(z;\kappa)]^{-1} - \lambda}\,\Psi_{z,l+\nu}(\kappa)\,. \tag{62}$$

This equation defines implicitly the operator $\hat{\mathcal{G}}_{l+\nu}(E)$.

Finally, Eq. (62) can be recast into the explicit form

$$\mathcal{G}_{l+\nu}(r'',r';E) = \int_0^\infty dz\,\frac{1}{[\eta_{l+\nu}(z;\kappa)]^{-1} - \lambda}\,\Psi_{z,l+\nu}(r'';\kappa)\Psi_{z,l+\nu}(r';\kappa)\,, \tag{63}$$

which stands for the Green's spectral representation (see Appendix). It should be noticed that the energy dependence of $\mathcal{G}_{l+\nu}(r'',r';E)$ arises from possibly both the eigenfunctions $\Psi_{z,l+\nu}(r;\kappa)$ and eigenvalues $\eta_{l+\nu}(z;\kappa)$.

The procedure outlined in the reconstruction of the previous paragraphs illustrates how the formal infinite summation can be implemented. However, a caveat is in order: Eq. (63) can only be turned into an explicit solution if the eigenvalue problem of Eq. (59) is solved first. As an alternative, the solution to Eq. (59) could be directly identified if a corresponding spectral representation

$$\mathcal{G}_{l+\nu}^{(0)}(r'',r';E) = \int_0^\infty dz\,\eta_{l+\nu}(z;\kappa)\,\Psi_{z,l+\nu}(r'';\kappa)\Psi_{z,l+\nu}(r';\kappa)\,. \tag{64}$$

were found. In short, the existence of an integral representation (64) implies directly the form (63) for the exact Green's function $\mathcal{G}_{l+\nu}(r'', r'; E)$.

For the remainder of this paper we will explore particular applications of this remarkable summation technique.

IV. QUANTUM-MECHANICAL PROPAGATOR FOR THE INVERSE SQUARE POTENTIAL

In this section we start a path-integral analysis of the inverse square potential

$$V(r) = -\frac{\hbar^2}{2M}\frac{\lambda}{r^2} \,, \tag{65}$$

which we conveniently rewrite in such a way that $\mathcal{V} = 1/r^2$ [cf. Eq. (53)] and λ be dimensionless; moreover, $\lambda < 0$ describes a repulsive potential, while $\lambda > 0$ describes an attractive interaction. Direct evaluation of Eq. (21) leads to complicated integrals and recursion relations that cannot be easily tamed (unlike the cases of a free particle and a harmonic oscillator). Instead, a judicious application of the method of infinite summation of perturbation theory leads to an exact analytical solution, which will constitute the main result of this section.

Before considering the complete solution, one may notice that Eqs. (27) and (28) describe physics of a free particle, for each angular momentum channel, and thereby suggest the following straightforward heuristic argument. First, one may consider the asymptotic behavior of the Bessel function,

$$\sqrt{2\pi z}\, e^{-z}\, I_p(z) \stackrel{(z\to\infty)}{\sim} 1 - \frac{(p^2 - 1/4)}{2z} \,, \tag{66}$$

in the limit $N \to \infty$, which according to Eq. (24) amounts to $z \to \infty$. Second, the asymptotics (66) can be applied to each factor in the pseudomeasure (23). Third, each exponential factor can be combined with and compared against a corresponding factor arising from the inverse square interaction. In conclusion, this shows that the only effect of adding an inverse square potential (65) to the propagator (21) is a shift in the angular momentum quantum number,

$$l + \nu \to s_l = \sqrt{(l+\nu)^2 - \lambda} \,. \tag{67}$$

Even though this replacement is straightforward in the Schrödinger formulation of the theory, its justification in the path-integral approach is far from obvious. Not surprisingly, the

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asymptotic argument has been called into question [6]. Thus, we will first refine the argument above and show how to confirm this conjecture (67) in a more satisfactory way.

A. Integral Representation of the Green's Function for the Inverse Square Potential

The derivation of the result of Eq. (67) can be completed in a number of equivalent ways. The most elegant route is based on direct transformations at the level of the energy Green's functions. For the inverse square potential (65), the perturbation expansion of Eqs. (55) and (56) reduces to the evaluation of Eqs. (57)–(63).

Remarkably, an integral representation of the form (64) is known, as first pointed in Ref. [15]; explicitly, it is the Kontorovich-Lebedev representation [26]

$$G_{l+\nu}^{(0)}(r'', r'; E) = -\frac{2M}{\hbar^2} \sqrt{r'r''}\, \mathcal{J}_{l+\nu}(\kappa r'', \kappa r'; 1)\,, \tag{68}$$

where

$$\mathcal{J}_p(\xi, \eta; \alpha) = \frac{2}{\pi^2} \int_0^\infty dz\, \frac{z \sinh(\pi z)}{(z^2 + p^2)^\alpha} K_{iz}(\xi) K_{iz}(\eta)\,. \tag{69}$$

In Eq. (68) the generalized function $\mathcal{J}_p(\xi, \eta; \alpha)$ reduces to the product of Bessel functions in Eq. (28),

$$\mathcal{J}_p(\xi, \eta; 1) = \sqrt{r'r''}\, \mathcal{G}_{l+\nu}^{(0)}(r, r'; E) = I_{l+\nu}(\kappa r_<) K_{l+\nu}(\kappa r_>)\,, \tag{70}$$

when $\alpha = 1$.

In the Kontorovich-Lebedev representation [26], which we review in the Appendix, the Dirac-normalized complete set of functions $\Psi_z(r; \kappa) = \sqrt{2z \sinh(\pi z)/(\pi^2 r)}\, K_{iz}(\kappa r)$ permits the identification of Eq. (69) [supplemented with Eq. (68)] with Eq. (63). Thus, Eq. (59) is realized with

$$\eta_{l+\nu}(z) = \frac{1}{z^2 + (l+\nu)^2}\,, \tag{71}$$

so that the eigenvalues (62) of $\hat{\mathcal{G}}_{l+\nu}(E)$ are

$$\frac{1}{[\eta_{l+\nu}(z)]^{-1} - \lambda} = \frac{1}{z^2 + s_l^2}\,. \tag{72}$$

It should be noticed that $\eta_{l+\nu}(z)$ is independent of the energy, while Ψ_z is independent of $(l + \nu)$; this is characteristic of the Kontorovich-Lebedev representation. Finally, the

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remarkable reconstruction (63) can be explicitly carried out,

$$
\begin{aligned}
G_{l+\nu}(r'',r';E|\lambda) &= -\frac{2M}{\hbar^2}\sqrt{r'r''}\sum_{n=0}^{\infty}\lambda^n \mathcal{J}_{l+\nu}(\kappa r'',\kappa r';n+1) \\
&= -\frac{2}{\pi^2}\frac{2M}{\hbar^2}\int_0^{\infty}dz\,\frac{z\sinh(\pi z)}{z^2+s_l^2}\,K_{iz}(\kappa r'')K_{iz}(\kappa r') \qquad (73)\\
&= -\frac{2M}{\hbar^2}\sqrt{r'r''}\,\mathcal{J}_{s_l}(\kappa r'',\kappa r';1)\,. \qquad (74)
\end{aligned}
$$

Equation (74) is identical in form with (68); thus, the replacement (67) is now proved within the path-integral formulation. In short, going back to Eq. (28),

$$
G_{l+\nu}(r'',r';E|\lambda)=G_{s_l}^{(0)}(r'',r';E)=-\frac{2M}{\hbar^2}\sqrt{r'r''}\,I_{s_l}(\kappa r_<)K_{s_l}(\kappa r_>)\,, \qquad (75)
$$

while its inverse Fourier transform is identical to $K_{s_l}^{(0)}(r'',r';T)$, so that [cf. (27)]

$$
K_{l+\nu}(r'',r';T|\lambda)=\frac{M}{i\hbar T}\sqrt{r'r''}\exp\left[\frac{iM}{2\hbar T}\left(r'^2+r''^2\right)\right]I_{s_l}\left(\frac{Mr'r''}{i\hbar T}\right)\,. \qquad (76)
$$

B. Nature of the Solution

There is only one apparent limitation in the above derivation: the geometric series involved in the infinite perturbation expansion is guaranteed to converge only for $|\lambda|<\lambda_l^{(*)}$, where $\lambda_l^{(*)}=(l+\nu)^2$. This condition has been regarded as an actual limitation [15]; however, as a restriction, it can be immediately lifted by noticing that the final expression (75) provides the desired analytic continuation in the complex λ plane.

Moreover, for each angular momentum state, the radius of convergence of the above series is set by the existence of a critical point $\lambda=\lambda_l^{(*)}$, at which the nature of the path integral for real λ changes. In fact, the integral representation (73) explicitly displays that there exist two fundamentally distinct regimes with respect to the coupling parameter λ (dependence which is encoded in s_l):

- Weak-coupling regime: $\lambda<\lambda_l^{(*)}$, including repulsive potentials.

  The order s_l of the Bessel functions is real and Eq. (75) has no singularities for real κ, showing that the system cannot sustain bound states—a manifestation of the scale invariance of the potential r^{-2}.

- Strong-coupling regime: $\lambda>\lambda_l^{(*)}$.

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The Bessel functions acquire an imaginary order $s_l = i\Theta_l$, where

$$\Theta_l = [\lambda - \lambda_l^{(*)}]^{1/2} \,, \tag{77}$$

and the negative-energy states form a continuous spectrum not bounded from below.

The pathology displayed in the strong-coupling spectrum can be avoided by the use of field-theory regularization and renormalization techniques, as shown in Refs. [9–11]. Accordingly, introducing a short-distance cutoff a, the resulting radial Green's function $G_{l+\nu}(r'', r'; E|\lambda; a)$ inherits the regular boundary condition

$$G_{l+\nu}(r'', r'; E|\lambda; a)|_{r''=a \text{ or } r'=a} = 0 \,. \tag{78}$$

However, the implementation of Eq. (78) is not straightforward in the path-integral formalism. The main difficulty encountered in a path-integral real-space renormalization with the Dirichlet boundary condition (78) lies in the proper implementation of the sum over all paths. A technique for dealing with this difficulty, which was originally introduced in Ref. [27], amounts to adding an infinite-strength repulsive delta-function potential $\sigma\delta(r-a)$. Therefore, we define the regularized radial energy Green's function $G_{l+\nu}(r'', r'; E|\lambda; a)$ as the limit $\sigma \to \infty$ of the more general Green's function $G_{l+\nu}(r'', r'; E|\lambda; a; \sigma)$ in the presence of the delta-function perturbation. We now turn our attention to this problem.

V. INVERSE SQUARE POTENTIAL IN THE PRESENCE OF A DELTA-FUNCTION INTERACTION

A. Computation of the Green's Function

We will now compute the general Green's function $G_{l+\nu}(r'', r'; E|\lambda; a; \sigma)$ in the presence of an interaction

$$V_{\text{total}}(r) = -\frac{\hbar^2}{2M}\frac{\lambda}{r^2} + \sigma\delta(r-a) \,. \tag{79}$$

This problem can be most effectively analyzed by treating it exactly to all orders as a delta-function perturbation to an inverse square potential. More precisely, the unperturbed action $S^{(0)}$ includes both the kinetic term and the inverse-square interaction, with their exact physics described by $G_{l+\nu}(r'', r'; E|\lambda)$, Eq. (75), or alternatively by $K_{l+\nu}(r'', r'; T|\lambda)$,

Eq. (76). In addition, the delta-function term $V(r) = \sigma\delta(r - a)$ is to be regarded as a perturbation to which the theory of Secs. II and III applies.

Then, going back to Eq. (52), each factor $\int_0^\infty dr_\alpha\, V(r_\alpha)$ is merely reduced to σ and carries the additional instruction that the replacement $r_\alpha \to a$ be made; then,

$$G_{l+\nu}^{(n)}\left(r'', r'; E\,|\,\lambda; a; \sigma\right) = \sigma^n\,\left[G_{l+\nu}(a, a; E|\lambda)\right]^{n-1}\,G_{l+\nu}(r'', a; E|\lambda)\,G_{l+\nu}(a, r'; E|\lambda) \qquad (80)$$

for $n \geq 1$, while the term of order zero distinctly remains $G_{l+\nu}(r'', r'; E|\lambda)$. The exact infinite summation of this series for finite σ leads to the familiar result [27]

$$G_{l+\nu}\left(r'', r'; E\,|\,\lambda; a; \sigma\right) = G_{l+\nu}(r'', r'; E|\lambda) - \frac{G_{l+\nu}(r'', a; E|\lambda)\,G_{l+\nu}(a, r'; E|\lambda)}{G_{l+\nu}(a, a; E|\lambda) - 1/\sigma}\,. \qquad (81)$$

It should be noticed that Eq. (81) describes the complete physics of a delta-function perturbation to *any* known problem with action $S^{(0)}$ and exactly described by $G_{l+\nu}(r'', r'; E|\lambda)$.

B.   Applications

The combined interaction (79) is of current interest, above and beyond its application to the regularization of the inverse square potential. Recent work in M-theory has led to a particular realization of this combined potential [28] and the use of Green's functions was advanced for further analysis [29], within a more general investigation of gravitation in our familiar four-dimensional world as arising from a higher-dimensional theory. Even though this example corresponds to a very specific model, it shows the usefulness of the examination of singular potentials with the techniques introduced in this paper.

Let us now briefly review the relevant example, which arises in the description of effective four-dimensional gravitational effects observed on a $(3 + 1)$-dimensional subspace, a 3-brane, embedded in a spacetime with five noncompact dimensions (AdS_5) [28]. The linearized tensor fluctuations of the metric are subject to a Kaluza-Klein reduction and assumed to have a dependence $h(x, y) = \psi(y)e^{p\cdot x}$ in terms of the coordinates x on the brane and the extra-dimensional coordinate y. The problem is then reduced to an *effective* one-dimensional Schrödinger equation with respect to the "wave function" $\psi(y)$ in terms of the extra-dimensional coordinate. Even though direct reduction leads to a complicated potential with respect to y, the transformation of variables $z = \mathrm{sgn}\,(y) \times (e^{k|y|} - 1)/k$,

$\hat{\psi}(z) = \psi(y)e^{k|y|/2}$ simplifies the effective Schrödinger problem to ($\hbar = 1$, $M = 1$)

$$\left\{ -\frac{1}{2}\partial_z^2 + \left[-\frac{\lambda}{2(|z| + a)^2} + \sigma\delta(z) \right] \right\} \hat{\psi}(z) = m^2\,\hat{\psi}(z)\,, \qquad (82)$$

with the following specific parameters:

$$\begin{aligned} \lambda &= -\frac{15}{4} \\ \sigma &= -3k \\ a &= \frac{1}{k}\,, \end{aligned} \qquad (83)$$

as dictated by the physics of the Kaluza-Klein reduction. More precisely, the additional coordinate change $\xi = |z| + a$, shows that Eq. (82) indeed describes an effective interaction of the form (79) with respect to the coordinate ξ. It should be noticed that the signs in this problem (attractive delta and repulsive inverse square potential) are just the opposite of the those needed for the regularization of the single inverse square potential, as discussed in the next section.

The effective dimensionality $D = 1$ ($\nu = -1/2$) of problem (82) implies that the only available channels are $l = 0$ and $l = 1$, so that $l + \nu = \mp 1/2$ respectively; from this and Eqs. (67) and (83), the corresponding order of the Bessel functions is $s_l = 2$. Even though the repulsive inverse square potential is incapable of producing bound states by itself, the additional presence of a one-dimensional attractive delta-function perturbation yields exactly one bound state [28]. This is interpreted as corresponding to a massless four-dimensional graviton—a fact that has been used to confirm the claim that the experimentally observed four-dimensional gravitational fields can arise through a hypothetical scenario of dimensional reduction from extra noncompact dimensions. Additional details on this problem and related applications are currently under investigation.

Parenthetically, a related and simple example of the application of these techniques is afforded by the two-dimensional delta-function potential $V(\mathbf{r}) = -\hbar^2 g\,\delta^{(2)}(\mathbf{r})/2M$, for which the propagator is also singular and calls for regularization. For example, using a real-space regulator a, one may replace $\delta^{(2)}(\mathbf{r})$ by $\delta(r - a)/2\pi a$. Then, selecting $\lambda = 0$, $\nu = 0$, and $\sigma = -\hbar^2 g/2M$ in Eq. (81) and identifying the pole(s), the regularized equation for the bound state in the s channel becomes $K_0(\kappa a) = 2\pi/g$, whose renormalized counterpart agrees with the known answer [30], as we have recently shown [31].

VI. REGULARIZATION OF THE INVERSE SQUARE POTENTIAL

We now turn our attention to the problem that was anticipated in Sec. IV: the real-space regularization of an inverse square potential with supercritical coupling. In this procedure, a short-distance regulator a is introduced and the boundary condition (78) is enforced as the $\sigma \to \infty$ limit of the Green's function $G_{l+\nu}(r'', r'; E|\lambda; a; \sigma)$ in the presence of the delta-function perturbation—the second term in Eq. (79).

Therefore, Eqs. (75) and (81) provide the desired regularized radial energy Green's function

$$G_{l+\nu}\left(r'', r'; E\,|\,\lambda; a\right) = -\frac{2M}{\hbar^2} \frac{\sqrt{r'r''}}{K_{s_l}(\kappa a)} \left[K_{s_l}(\kappa a)I_{s_l}(\kappa r_<) - I_{s_l}(\kappa a)K_{s_l}(\kappa r_<)\right]K_{s_l}(\kappa r_>) , \quad (84)$$

where $\kappa = \sqrt{-2ME}/\hbar$ [cf. Eq. (28)]. Equation (84) is in perfect agreement with the result from the operator approach to a Green's function: $G(r'', r'; E) = u_<(r_<)u_>(r_>)/pW[u_<, u_>]$, where $p = \hbar^2/2M$, while $u_<(r)$ and $u_>(r)$ are the solutions satisfying the boundary condition at $r = a$ and at infinity [32].

The poles of Eq. (84), which are implicitly given by

$$K_{s_l}(\kappa a) = 0 , \quad (85)$$

yield the bound-state sector of the theory. The energy levels can be derived by specializing to the case when a is small, in which case the small-argument expansion of the modified Bessel function of the second kind becomes [10, 33]

$$K_{i\Theta_l}(z) \overset{(z\to 0)}{\sim} -\sqrt{\frac{\pi}{\Theta_l \sinh(\pi\Theta_l)}} \sin\left[\Theta_l \ln\left(\frac{z}{2}\right) - \delta_{\Theta_l}\right]\left[1 + O\left(z^2\right)\right] , \quad (86)$$

in which δ_{Θ_l} is the phase of $\Gamma(1 + i\Theta_l)$. In particular, Eq. (86) has an infinite set of zeros when the order of the modified Bessel function is imaginary; these zeros are

$$z_n = 2\,e^{(\delta_{\Theta_l} - n\pi)/\Theta_l} \quad (87)$$

[up to a correction factor $1 + O(z_n^2/\Theta_l)$], where n is an integer. Furthermore, with the assumption that $z_n \ll 1$ and $\Theta_l \geq 0$, it follows that $(-n) < 0$, whence $n = 1, 2, 3, \ldots$. Parenthetically, $z_n \ll 1$ only if $\Theta_l \ll 1$, so that $\delta_{\Theta_l} = -\gamma\Theta_l + O(\Theta_l^2)$ (with γ being the Euler-Mascheroni constant). This argument shows that the energy levels are given by

$$E_{n_r l} = -\frac{2\hbar^2 e^{-\gamma}}{Ma^2} \exp\left(-\frac{2\pi n_r}{\Theta_l}\right) , \quad (88)$$

in which $n = n_r$ is the usual radial quantum number.

The regularization of Eq. (85) provides the foundation for the next step: renormalization. This final step may be implemented by demanding the dependence of the coupling with respect to the regulator; from Eq. (77) this implies the dependence $\Theta_l = \Theta_l(a)$ in the limit $a \to 0$ [34], as in Refs. [9–11]. For example, when this procedure is applied to the regularized ground state, the required relation becomes

$$ - g^{(0)} = \frac{2\pi}{\Theta_{(gs)}(a)} + 2 \ln\left(\frac{\mu a}{2}\right) + 2\gamma, \tag{89} $$

where μ is an arbitrary renormalization scale with dimensions of inverse length and $g^{(0)}$ is an arbitrary finite part associated with the coupling, such that

$$ E_{(gs)} = -\frac{\hbar^2 \mu^2}{2M} \exp\left[g^{(0)}\right]. \tag{90} $$

The ground-state wave function is obtained in the limit $\Theta_{(gs)}(a) \xrightarrow{(a \to 0)} 0^+$, so that, from Eqs. (17) and (18),

$$ \Psi_{(gs)}(\mathbf{r}) = \sqrt{\Gamma\left(\frac{D}{2}\right)\left(\frac{\mu^2}{\pi}\right)^{D/2} \frac{K_0(\mu r)}{(\mu r)^{D/2-1}}}. \tag{91} $$

The renormalization procedure described above leads to the emergence of an arbitrary dimensional scale—phenomenon known as dimensional transmutation—and violates the manifest SO(2,1) invariance of the theory [17, 35–37]. This is an instance of an established quantum anomaly, which manifests itself in the three-dimensional molecular realm for the interaction between polar molecules and electrons [17].

Finally, the scattering sector of the theory can be analyzed in a similar way, with the Bessel functions in Eq. (84) replaced as follows: $I_s(\kappa r) \to (-i)^s J_s(kr)$ and $K_s(\kappa r) \to \pi i^{s+1} H_s^{(1)}(kr)/2$, and the S-matrix derived with the formulation of Ref. [38]. These results, as well as additional properties of the inverse square potential and other singular interactions, will be presented elsewhere.

VII. QUANTUM FIELD THEORY

Some comments on the quantum field theory case are now in order. The connection to this work is twofold:

(i) The emphasis on singular potentials that we have adopted in this paper can be traced fundamentally to their field-theory origin. This explicit connection is illustrated below, in the final paragraph of this section.

(ii) The approach initiated in this paper provides the underlying philosophy and hopefully a partial set of ingredients for the more general program of bound states in quantum field theory. This generalization is currently in progress.

In particular, the definitions of Sec. II A can be adjusted as follows. Let us consider the path integral

$$\langle \phi_2(\mathbf{x}), t_2 \,|\, \phi_1(\mathbf{x}), t_1 \rangle = \int_{\phi(\mathbf{x}, t_1)=\phi_1(\mathbf{x})}^{\phi(\mathbf{x}, t_2)=\phi_2(\mathbf{x})} \mathcal{D}\phi \, \exp\left\{ \frac{i}{\hbar} S[\phi] \right\} \tag{92}$$

of the field $\phi(\mathbf{x})$ between the states $|\phi_1(\mathbf{x}, t_1)\rangle$ and $|\phi_2(\mathbf{x}, t_2)\rangle$, corresponding to the propagator

$$\langle \phi_2(\mathbf{x}), t_2 \,|\, \phi_1(\mathbf{x}), t_1 \rangle = \left\langle \phi_2(\mathbf{x}) \left| \hat{T} \exp\left[-\frac{i}{\hbar} \int_{t_1}^{t_2} \hat{H} dt \right] \right| \phi_1(\mathbf{x}) \right\rangle, \tag{93}$$

with $\hat{T}$ being again the time-ordering operator and $\hat{H}$ the Hamiltonian. For time-independent Hamiltonians the "energy propagator" is defined to be

$$\begin{aligned}
\left(\phi_2(\mathbf{x}) \,|\, \phi_1(\mathbf{x}) \right)_E &= \frac{1}{i\hbar} \int_{t_1}^{\infty} dt_2 \, \langle \phi_2(\mathbf{x}), t_2 | \phi_1(\mathbf{x}), t_1 \rangle \, e^{iE(t_2-t_1)/\hbar} \\
&= \left\langle \phi_2(\mathbf{x}) \left| \left(E - \hat{H} + i\epsilon \right)^{-1} \right| \phi_1(\mathbf{x}) \right\rangle
\end{aligned} \tag{94}$$

(with $i\epsilon$ being a small positive imaginary part), which admits a spectral representation

$$\left(\phi_2(\mathbf{x}) \,|\, \phi_1(\mathbf{x}) \right)_E = \sum_n \frac{\Psi_n[\phi_2(\mathbf{x})] \, \Psi_n^*[\phi_1(\mathbf{x})]}{E - E_n + i\epsilon} + \int d\alpha \, \frac{\Psi_\alpha[\phi_2(\mathbf{x})] \, \Psi_\alpha^*[\phi_1(\mathbf{x})]}{E - E_\alpha + i\epsilon} \tag{95}$$

and permits, in principle, the identification of bound states and scattering states, as well as the corresponding wave functionals.

A subtlety arises in the usual description of bound states at low energies, which requires a nonrelativistic (nr) reduction to be performed in one of the following ways: (i) application of the nr limit to the original path integral (92), followed by evaluation of the Fourier transform, to be subsequently expanded as in (95); (ii) application of the nr limit at the level of Eq. (95). It is not obvious that procedures (i) and (ii) are equivalent. In nuclear physics at low energies one may wish to integrate out the light field (e.g., pions) and describe the dynamics in terms of the heavy field only (i.e., nucleons). Issues about the order in which to take the nr limit are also present in this case. Regardless of the route taken, the appearance of singular potentials

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is a generic feature of these nr reductions from field theory to quantum mechanics [39, 40]. The proper treatment of these potentials is notoriously difficult and requires regularization and renormalization of the corresponding propagator. This particular problem has been addressed for the inverse square potential in Sec. VI.

An intriguing application of these ideas can be found in the recent literature [41] in relation to the study of bound states for the Yukawa model,

$$\mathcal{L}_{\text{int}} = g\bar{\Psi}\Psi\varphi \,, \tag{96}$$

where Ψ represents fermions and φ the scalar interaction. For two-fermion wave functions of total angular momentum $J = 0^+$, and within a covariantized light-cone technique, the stability of bound states can be assessed by the asymptotics of an effective wave equation that simulates a nonrelativistic inverse square potential. Additional subtleties of this problem arising from the renormalized strong-coupling sector of the theory are currently under investigation.

VIII. CONCLUSIONS

In summary, we have formulated the general outline of a program for the evaluation of quantum-mechanical propagators and energy Green's functions. We have also thoroughly examined the inverse square potential within such path-integral framework. Our analysis included renormalization *à la* field theory in the (strong) supercritical regime, as well as the inclusion of an additional delta-function interaction. The general technique as well as the particular examples suggest that:

(i) The treatment of singular potentials—and of bound states in general—is most efficiently accomplished by the use of the Fourier-transformed or energy Green's function $G(E)$.

(ii) Infinite summations and resummations in the spirit of perturbation theory capture the required nonperturbative behavior associated with the bound-state sector of the theory.

(iii) Proper analytic continuations are needed in certain regimes.

(iv) The effective-field-theory program, which leads to singular potentials, requires renormalization in a quantum-mechanical setting—renormalization that, in principle, could be implemented with techniques similar to the ones presented in this paper.

Extensions of this generic program will be presented elsewhere.

Appendix: Formal Operator Structure of the Perturbation Expansion

In this appendix we summarize the formal algebraic structure of the operator expansions presented in Sec. III C. In addition, we review the necessary ingredients of the Kontorovich-Lebedev transform, properly adjusted to the notation and goals of this paper, and with emphasis on the results of Secs. III C and IV A.

A normalized continuous basis for the space of square integrable functions over the interval $\mathcal{I} \in \mathbb{R}$ is provided by the set of functions $\{\Psi_z(q)\}_{z \in \mathcal{J}}$ that satisfy the orthonormality condition

$$\int_{\mathcal{I}} dq\, \Psi_{z''}^*(q)\, \Psi_{z'}(q) = \delta(z'' - z') \tag{A.1}$$

and the completeness relation

$$\int_{\mathcal{J}} dz\, \Psi_z(q)\, \Psi_z^*(q') = \delta(q - q')\,, \tag{A.2}$$

with the continuous variable z defined over an interval $\mathcal{J} \in \mathbb{R}$. A particular set $\{\Psi_z(q)\}_{z \in \mathcal{J}}$ can be constructed by selecting the eigenbasis associated with an appropriate self-adjoint operator, with properly chosen boundary conditions. The mathematical theory required for such bases, which is extremely subtle, should be studied carefully for every specific case, and no attempt is made to develop a rigorous presentation in this paper. Within that operational framework, we adopt the usual Dirac notation, which reproduces the required formal algebraic structure of Eqs. (A.1) and (A.2) from

$$\langle \Psi_{z''} | \Psi_{z'} \rangle = \delta(z'' - z') \tag{A.3}$$

and

$$\int_{\mathcal{J}} dz\, |\Psi_z\rangle \langle \Psi_z| = \mathbb{1}\,. \tag{A.4}$$

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In particular, the basis $\{|q\rangle\}$ provides direct contact with the functions $\Psi_z(q) \equiv \langle q|\Psi_z\rangle$. These are the functions used in the expansions of Sec. III C, where $q \equiv r$ represents the radial variable.

The most important results of Secs. III C and IV A rely on the properties of operators. With that purpose in mind, an operator $\hat{A}$ is represented by the "continuous matrix" $A(q'', q') = \langle q''|A|q'\rangle$ in the basis $\{|q\rangle\}$. More generally, $\hat{A}$ admits the representation $\langle \Psi_{z''}|A|\Psi_{z'}\rangle$ in the $\{|\Psi_z\rangle\}_{z\in\mathcal{J}}$, in terms of which the sesquilinear expansion

$$\langle q''|A|q'\rangle = \int_{\mathcal{J}} dz'' \int_{\mathcal{J}} dz'\, \Psi_{z''}(q'')\, \langle \Psi_{z''}|A|\Psi_{z'}\rangle\, \Psi_{z'}^*(q') \tag{A.5}$$

directly follows by double insertion of the completeness identity (A.4).

Equation (A.5) is further simplified for the particular case in which $|\Psi_{z'}\rangle$ represents the eigenbasis of a self-adjoint operator $\hat{A}$, with eigenvalues $a(z)$. In that case,

$$\langle q''|A|q'\rangle = \int_{\mathcal{J}} dz\, a(z)\, \Psi_z(q'')\, \Psi_{z'}^*(q') \tag{A.6}$$

is the required spectral representation of the operator, which we have directly applied, for example, to Eqs. (63), (64), and (73).

The integral transform of the function $f(q)$ by the kernel $K(z, q)$ is defined by

$$\mathcal{T}\{f(q); K(z,q)\}(z) \equiv \tilde{f} = \int_{\mathcal{I}} dq\, K(z,q) f(q)\,, \tag{A.7}$$

with appropriate conditions required for the convergence of the integrals involved. Of particular interest for the derivations of Secs. III C and IV A is the class of integral transforms that arise from generalized bases; specifically, given the basis $\{|\Psi_z\rangle\}_{z\in\mathcal{J}}$, the associated transform is defined by

$$\mathcal{T}\{f(q); K(z,q)\}(z) = \int_{\mathcal{J}} dq\, \Psi_z^*(q)\, f(q)\,, \tag{A.8}$$

which amounts to $K(z, q) \equiv \Psi_z^*(q)$. Equation (A.8) is just a particular set of "components" of the vector $|f\rangle$, as can be seen with the Dirac notation

$$\mathcal{T}\{f(q); K(z,q)\}(z) = \langle \Psi_z|f\rangle\,, \tag{A.9}$$

by insertion of the completeness relation for the $|q\rangle$ basis. The abbreviated notation $\tilde{f}(z) = \langle z|f\rangle$ highlights that this class of integral transforms amounts to a mere change of basis in Hilbert space—the analogue of the "passive" view of a coordinate transformation.

Reciprocally, the integral transform (A.8) can be used to reproduce the original function by means of an inversion identity

$$f(q) = \int_{\mathcal{J}} dz \, \Psi_z(q) \, \tilde{f}(z) \,, \tag{A.10}$$

which follows by insertion of the completeness relation for the generalized basis (A.2). A few of the most common examples of this kind of integral transform are provided by the following partial list of transformation kernels or bases (in 1D): (i) exponential Fourier transforms, $\Psi_z(q) = (2\pi)^{-1/2} e^{\pm iqz}$; (ii) trigonometric Fourier transforms, $\Psi_z(q) = \sqrt{2/\pi} \, \tau(qz)$, with $\tau = \sin$ or $\tau = \cos$; (iii) Hankel (Fourier-Bessel) transforms, $\Psi_z(q) = (qz)^{1/2} J_\mu(qz)$; etc. However, this general formal structure is of interest to gain familiarity with more exotic cases, such as the Kontorovich-Lebedev transform, which is central to our analysis of the inverse square potential in Sec .IV A.

The Kontorovich-Lebedev representation [26], is based on the modified Bessel function of the second kind with imaginary order $K_{iz}(q)$, with the the relevant interval being the real half-line $\mathcal{I} = [0, \infty)$. The notation $q \equiv \kappa r$ proves convenient for direct comparison with the equations of Sec. IV A; it is noteworthy that, due to a simple scaling argument (equivalent to scale invariance of the inverse square potential), the corresponding Dirac-normalized complete set of functions is

$$\Psi_z(r; \kappa) = \sqrt{\frac{2z \sinh(\pi z)}{\pi^2 r}} \, K_{iz}(\kappa r) \,. \tag{A.11}$$

An important property of the Bessel functions $K_{iz}(q)$ for real variables q and z is that $K_{iz}^*(q) = K_{iz}(q)$, i.e., it is real. The orthonormality relation (A.1) of the functions $\{\Psi_z(r)\}_{z \in \mathcal{J}}$, with $\mathcal{J} = [0, \infty)$, amounts to the integral identity

$$\int_0^\infty \frac{dr}{r} K_{iz''}(\kappa r) K_{iz'}(\kappa r) = \frac{\pi^2}{2z \sinh(\pi z)} \delta(z'' - z') \,, \tag{A.12}$$

which can be verified from the integral of the expression [42]

$$K_{iz''}(x) K_{iz'}(x) = 2 \int_0^\infty dt \, K_{i(z'+z'')}(2x \cosh t) \cos[(z''-z') t] \,, \tag{A.13}$$

with respect to x, followed by an exchange of the order of integration and explicit integration of the remaining expression [24], with an appropriate analytic continuation. Finally, completeness is just equivalent to the Kontorovich-Lebedev inversion identity,

$$\frac{2}{\pi^2} \int_0^\infty dz \, z \sinh(\pi z) K_{iz}(x) dz \int_0^\infty \frac{dy}{y} K_{iz}(y) f(y) = f(x) \tag{A.14}$$

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(see Ref. [26]) for functions $f(x)$ defined on the positive real half-line with appropriate conditions required for convergence.

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