A Green’s function approach is presented for the $D$-dimensional inverse square potential in quantum mechanics. This approach is implemented by the introduction of hyperspherical coordinates and the use of a real-space regulator in the regularized version of the model. The application of Sturm-Liouville theory yields a closed expression for the radial energy Green’s function. Finally, the equivalence with a recent path-integral treatment of the same problem is explicitly shown.

1. Introduction

The use of path integrals for the analysis of the bound-state and scattering sectors in quantum mechanics has significantly advanced in the past three decades. However, much work remains to be done, a situation that is particularly evident for the case of singular potentials. Among these, the contact interactions and the inverse square potential stand out; these problems have been the subject of active research in the past few years, mainly through the direct use of the Schrödinger equation combined with appropriate regularization and renormalization analyses à la field theory. Recently we have started a program centered on the use of path integrals for a systematic study of bound states and of the connection between field theory and quantum mechanics. We expect that our approach may shed light on the formidable problem posed by bound states in quantum field theory. In addition to introducing a technique of infinite summations of perturbation theory, we have specifically found analytic solutions for the two most outstanding singular interactions: the inverse square potential and the two-dimensional delta-function interaction.

In this paper we now investigate the quantum-mechanical properties of the inverse square potential from a complementary viewpoint, using an intrinsically non-
perturbative operator approach. This is accomplished by directly considering the problem associated with the energy Green’s function $G(E)$, defined as the Fourier transform of the path-integral propagator $K(T)$ [multiplied by the Heaviside function $\theta(T)$]. The Green’s function is then computed by solving a Sturm-Liouville problem in real space. Our final results are in complete agreement with the ones we obtained earlier by means of a path-integral perturbative approach. More precisely, we explicitly show that both approaches reproduce identical energy Green’s functions.

The relevance of this computation is highlighted by its recent application to a simple realization of a quantum anomaly in Nature: the interaction of an electron with a polar molecule. As shown in Ref. 23, the scale symmetry properties of the inverse square potential are inherited by the full-fledged dipole potential describing the physics of this system—electron binding occurs for a sufficiently strong coupling (dipole moment) and this amounts to quantum mechanical symmetry breaking. Our calculations in this paper provide additional support for this remarkable and unusual result. This mechanism is further analyzed in Sec. 4.

2. General Framework

The path-integral treatment for a $D$-dimensional nonrelativistic particle is based on the quantum-mechanical propagator

$$K_D(r'',r';t'',t') = \lim_{N \to \infty} \left( \frac{M}{2\pi i\hbar} \right)^{D/2} \prod_{k=1}^{N-1} \int_{\mathbb{R}^D} d^D r_k \ e^{iS(N)/\hbar}.$$  \hspace{1cm} (1)

Equation (1) has been explicitly formulated in Cartesian coordinates by means of a time lattice $t_j = t' + j\epsilon$ [where $\epsilon = (t'' - t')/N$, with $j = 0, \ldots, N$, while $t_0 \equiv t'$ and $t_N \equiv t''$], such that $r_j = r(t_j)$, with the end points being $r_0 \equiv r'$ and $r_N \equiv r''$. The corresponding discrete action in Eq. (1) is $S(N) = \sum_{j=0}^{N-1} S_j^{(N)}$, with $S_j^{(N)} = M(r_{j+1} - r_j)^2/2\epsilon - eV(r_j, t_j)$, for a particle of mass $M$ subject to a potential $V(r, t)$. The connection with the operator approach is established by means of

$$K_D(r'',r';t'',t') = \left\langle r'' \left| \hat{T} \exp \left[ -\frac{i}{\hbar} \int_{t'}^{t''} \hat{H} dt \right] \right| r' \right\rangle,$$ \hspace{1cm} (2)

where $\hat{T}$ is the time-ordering operator and $\hat{H}$ is the Hamiltonian. For a time-independent Hamiltonian, the dependence of Eq. (2) with respect to the times $t'$ and $t''$ is only through the time difference $T = t'' - t'$. For this all-important case, the energy Green’s function is then defined as a Fourier transform of the Green’s function obtained from (1)-(2) by multiplication with the Heaviside function $\theta(T)$, i.e.,

$$G_D(r'',r';E) = \frac{1}{i\hbar} \int_0^\infty dT e^{iE T/\hbar} K_D(r'',r';t'',t').$$ \hspace{1cm} (3)
Regularized Green's Function/Inverse Square Potential

Equations (2) and (3) establish the operator form of the energy Green's function in its configuration-space representation, which explicitly becomes

\[
G_D(r'', r'; E) = \left< r'' \left| \left( E - \hat{H} + i\epsilon \right)^{-1} \right| r' \right>, \tag{4}
\]

where \( i\epsilon = i0^+ \) is a small imaginary part. The operator structure of Eq. (3) implies the differential equation

\[
\left\{ \nabla^2 + \frac{2M}{\hbar^2} |E - V(r')| \right\} G_D(r'', r'; E) = \delta(r'' - r'), \tag{5}
\]

in which we have conveniently defined the rescaled Green’s function

\[
G_D(r'', r'; E) = \frac{\hbar^2}{2M} G_D(r'', r'; E). \tag{6}
\]

For the particular case of a central potential, Eq. (5) can be solved by separation of variables. This procedure can be systematically implemented by considering a complete set of angular functions, the \( D \)-dimensional hyperspherical harmonics \( Y_{lm}(\Omega) \), for which \( l \) is the angular momentum quantum number and \( m = 0, \ldots, d_l \), with \( d_l = (2l + D - 2)(l + D - 3)!/(D - 2)! \). Then, the partial-wave expansion

\[
G_D(r'', r'; E) = (r''r')^{-(D-1)/2} \sum_{l=0}^\infty \sum_{m=1}^{d_l} Y_{lm}(\Omega'')Y_{lm}^*(\Omega') G_{l+\nu}(r'', r'; E) \tag{7}
\]

implicitly defines the radial energy Green’s function \( G_{l+\nu}(r'', r'; E) \) for each angular momentum channel \( l \) and dimensionality \( D = 2(\nu + 1) \). Equation (7) has been written to explicitly display the property of interdimensional dependence, except for the scale prefactors \( (r''r')^{-(D-1)/2} \), the only dependence of \( G_D(r'', r'; E) \) upon the dimensionality \( D \) is through the combination \( l + \nu \), and this information is conveyed by the function \( G_{l+\nu}(r'', r'; E) \). Likewise we define a rescaled radial Green’s function \( G_{l+\nu}(r'', r'; E) \) from the expansion of \( G_D(r'', r'; E) \), just as in (6)—or alternatively, by directly enforcing the analogue of Eq. (5). Then, substitution of Eq. (7) in (5) yields the radial differential equation

\[
\left\{ \frac{d^2}{dr''^2} + \frac{2M}{\hbar^2} [E - V(r')] - \frac{(l + \nu)^2 - 1/4}{r''^2} \right\} G_{l+\nu}(r'', r'; E) = \delta(r'' - r'), \tag{8}
\]

which stands for a particular case of the Sturm-Liouville Green’s function problem:

\[
\left\{ \frac{d}{dr'} \left[ p(r') \frac{d}{dr'} \right] + \eta + q(r') \right\} G(r'', r'; E) = \delta(r'' - r'), \tag{9}
\]

with \( p(r) \equiv 1, \eta = 2M E/\hbar^2, \) and \( q(r) = -2MV_{\text{eff}}(r)/\hbar^2 \); here \( V_{\text{eff}}(r) \) includes, in addition to the potential \( V(r) \), the centrifugal barrier displayed as the last term on the right-hand side of Eq. (8).
Equation (11) can be solved by applying the following standard technique. Let \( u_{l,\nu}^{(\ <)}(r) \) and \( u_{l,\nu}^{(\ >)}(r) \) be the particular solutions to the corresponding homogeneous differential equation

\[
\left\{ \frac{d}{dr} \left[ p(r) \frac{d}{dr} \right] + \eta + q(r) \right\} u_{l,\nu}(r) = 0 ,
\]

subject to the appropriate boundary conditions: \( u_{l,\nu}^{(\ <)}(r) \) at the left boundary and \( u_{l,\nu}^{(\ >)}(r) \) at the right boundary. Then, the Green’s function is given by

\[
G_{l+\nu}(r'', r'; E) = \frac{u_{l,\nu}^{(\ <)}(r'')u_{l,\nu}^{(\ >)}(r')}{{p(r')} W \left\{ u_{l,\nu}^{(\ <)}, u_{l,\nu}^{(\ >)} \right\} (r')},
\]

where \( r_<(r_>) \) is the smaller (larger) of \( r' \) and \( r'' \), while \( W \left\{ u_{l,\nu}^{(\ <)}, u_{l,\nu}^{(\ >)} \right\} (r) \) is the Wronskian of \( u_{l,\nu}^{(\ <)}(r) \) and \( u_{l,\nu}^{(\ >)}(r) \).

Solving Eq. (11) requires specific knowledge of the potential and has to be dealt with on a case-by-case basis. We now turn our attention to the advertised problem: the inverse square potential.

3. Green’s Function for the Inverse Square Potential

For the case of an inverse square potential, we conveniently write

\[
V(r) = -\frac{\hbar^2}{2M} \frac{\lambda}{r^2} ,
\]

so that

\[
\left[ \frac{d^2}{dr^2} + \frac{\eta - \frac{(l + \nu)^2}{r^2} - \lambda - 1/4}{r^2} \right] G_{l+\nu}(r'', r'; E) = \delta(r'' - r') .
\]

As a particular case of the Sturm-Liouville problem (11), Eq. (13) can be solved by introducing the functions \( u_{l,\nu}^{(\ <)}(r) \) and \( u_{l,\nu}^{(\ >)}(r) \) that satisfy the corresponding homogeneous differential equation

\[
\left[ \frac{d^2}{dr^2} + \frac{\eta - \frac{(l + \nu)^2}{r^2} - \lambda - 1/4}{r^2} \right] u_{l,\nu}(r) = 0 ,
\]

along with the boundary conditions outlined in Sec. 2. Equation (14) is immediately recognized to have solutions of the generic form

\[
u_{l,\nu}(r) = \sqrt{r} Z_{s_{l}}(\sqrt{\eta}r) ,
\]

where \( Z_{s_{l}}(z) \) represents an appropriate linear combination of Bessel functions of order

\[
sl = \sqrt{\lambda^{(s)} - \lambda} ,
\]
with
\[ \lambda_1^{(s)} = (l + \nu)^2 . \] (17)

Simple inspection of Eqs. (13) and (14) shows that the only effect of adding an inverse square potential \( V(r) = -\hbar^2 \lambda/2Mr^2 \) to a free particle is a shift in the angular momentum quantum number,
\[ l + \nu \rightarrow s_l = \sqrt{(l + \nu)^2 - \lambda} . \] (18)

This analysis shows that \( \lambda_1^{(s)} \) in Eq. (17) plays the role of a critical coupling, i.e., the nature of the solutions changes abruptly around the value \( \lambda = \lambda_1^{(s)} \), for any state with angular momentum \( l \).

Thus, \( \lambda_1^{(s)} \) represents the threshold separating the two coupling-strength regimes:
- subcritical or weak coupling, \( \lambda < \lambda_1^{(s)} \) (i.e., real \( s_l \));
- supercritical or strong coupling, \( \lambda > \lambda_1^{(s)} \) (i.e., imaginary \( s_l \)).

In the latter case the order can be rewritten as \( s_l = i \Theta_l \), with a real parameter
\[ \Theta_l = \sqrt{\lambda - \lambda_1^{(s)}} . \] (19)

Classification of the nature of the solutions can be fully accomplished by also considering the values of the energy \( E = \hbar^2 \eta/2M \):

(i) scattering states amount to \( \eta = k^2 > 0 \), for which the Bessel functions in Eq. (15) have real argument \( kr \);
(ii) bound states amount to \( \eta = -\kappa^2 < 0 \), for which the Bessel functions have imaginary argument \( kr = i\kappa r \).

As a result, the solutions (15) fall into one of the following four families:

(i) subcritical bound-state sector:
\[ u_{l,\nu}(r)/\sqrt{r} = \left\{ I_{s_l}(\kappa r), K_{s_l}(\kappa r) \right\} ; \]

(ii) subcritical scattering sector
\[ u_{l,\nu}(r)/\sqrt{r} = \left\{ H_{s_l}^{(1)}(kr), H_{s_l}^{(2)}(kr) \right\} ; \]

(iii) supercritical bound-state sector:
\[ u_{l,\nu}(r)/\sqrt{r} = \left\{ I_{i\Theta_l}(\kappa r), K_{i\Theta_l}(\kappa r) \right\} ; \]

(iv) supercritical scattering sector:
\[ u_{l,\nu}(r)/\sqrt{r} = \left\{ H_{i\Theta_l}^{(1)}(kr), H_{i\Theta_l}^{(2)}(kr) \right\} . \]
Here the symbol $\{,\}$ represents a linear combination and $H^{(1,2)}_s(z)$ stand for the Hankel functions of the first and second kinds, whereas $I_s(z)$ and $K_s(z)$ stand for the modified Bessel functions of the first and second kinds, respectively.

The analysis of Ref. 15 applies almost verbatim to the Green’s function formula, with the result that regularization is only needed in the supercritical coupling regime. However, in this paper—just as in Refs. 12 and 13—we regularize the inverse square potential by introducing a real-space regulator $a$, a procedure that is different from the dimensional regularization of Ref. 15. The introduction of a regulator is necessary for strong coupling because the inverse square potential fails to provide a discriminating boundary condition at the origin. Thus, this singular behavior leads to the emergence of a scale—a behavior known as dimensional transmutation.

In some sense, the key to a successful regularization procedure is the restoration of a sensible boundary condition at the origin. In particular, a real-space regulator allows one to restore the usual homogeneous boundary condition, but now displaced away from the origin to a radial position $r = a$. In short, the boundary conditions satisfied by the Green’s function are:

- boundary condition at infinity,
  \[ u^{(>)}_{l,\nu}(r) \xrightarrow{r \to \infty} 0 ; \] (20)
- boundary condition at $r = a$,
  \[ u^{(<)}_{l,\nu}(a) = 0 . \] (21)

In what follows and as anticipated for the supercritical regime, $s_l = i\Theta_l$, with $\Theta_l$ real and given by Eq. (19). From the behavior of Bessel functions and the boundary conditions, one concludes that, for the bound-state sector of the theory,

\[ u^{(<)}_{l,\nu}(r) \propto \sqrt{r} \left[ K_{s_l}(\kappa a)I_{s_l}(\kappa r) - I_{s_l}(\kappa a)K_{s_l}(\kappa r) \right] \] (22)

[which satisfies condition (21)] and

\[ u^{(>)}_{l,\nu}(r) \propto \sqrt{r} K_{s_l}(\kappa r) \] (23)

[which satisfies condition (20)]. In addition, from the well-known properties of the Sturm-Liouville equation, the Wronskian of any two Bessel functions $Z(z)$ is proportional to $1/z$; for the problem at hand, it suffices to know (for example, from the small-argument behavior of the Bessel functions) that $W \{K_s(z), I_s(z)\} = 1/z$. Then, Eq. (8) yields straightforwardly the desired regularized radial energy Green’s function

\[ G_{l+\nu}(r''; r'; E| \lambda; a) = -\frac{2M}{\hbar^2} \sqrt{r''r'} \frac{K_{i\Theta_l}(\kappa r_>)}{K_{i\Theta_l}(\kappa a)} \times \left[ K_{i\Theta_l}(\kappa a)I_{i\Theta_l}(\kappa r_<) - I_{i\Theta_l}(\kappa a)K_{i\Theta_l}(\kappa r_<) \right] , \] (24)
Regularized Green’s Function/Inverse Square Potential

with \( \kappa = \sqrt{-2ME/\hbar} \).

Analysis of the scattering sector requires an analytic continuation to positive energies, with a replacement of the Bessel functions in Eq. (24) as follows: \( I_s(\kappa r) \rightarrow (-i)^s J_s(\kappa r) \) and \( K_s(\kappa r) \rightarrow \pi i^{s+1} H^{(1)}_s(\kappa r)/2 \); then,

\[
G_{l+\nu}(r'', r'; E|\lambda; a) = -\frac{2M}{\hbar^2} \frac{\pi i}{2} \sqrt{r''r'} \frac{H^{(1)}_{ik}\Theta_l(ka)}{H^{(1)}_{ik}\Theta_l(\kappa a)} \times \left[ H^{(1)}_{ik}\Theta_l(ka)J_{i\Theta_l}(kr_<) - J_{i\Theta_l}(ka)H^{(1)}_{ik}\Theta_l(ka) \right],
\]

Equations (24) and (25) provide the solution to our problem because the energy Green’s functions summarize all the physical information about bound states and scattering. Indeed, Eq. (24) is identical to the corresponding formula recently found in Ref. [17]. This completes the proof of the equivalence between the perturbative method of Ref. [17] and the nonperturbative approach of this paper.

4. Renormalization, Anomalies, and Conclusions

The analysis that follows from Eq. (24) is identical to that of Ref. [17], which we summarize here for completeness. The bound-state sector of the theory is determined by the poles of Eq. (24), which provide the implicit solutions of the equation \( K_s(\kappa a) = 0 \). This equation provides no bound states in the subcritical regime, but the imaginary index \( s_i = i\Theta_i \) changes the nature of the Bessel function and leads to bound states in the supercritical regime. Then, as \( a \) is just a real-space regulator, attention needs to be focused only upon the limiting behavior for small \( a \); consequently, the energy levels become \( E_{l+_n} = -(2e^{-7/a})^2 \exp(-2\pi n_r/\Theta_l) \) (with \( n = n_r \) being the radial quantum number). This result, properly renormalized [with \( \Theta_l = \Theta_l(a) \) in the limit \( a \rightarrow 0 \)], reproduces the known solution of the path-integral approach\([17]\) and of the Hamiltonian operator approach\([12,13,15]\).

A remarkable property of this solution is the emergence of an arbitrary dimensional scale, within a theory that is devoid of dimensional scales at the level of the Lagrangian—the phenomenon of dimensional transmutation.\([29]\)

An even more illuminating approach to this scale problem is provided by a general analysis of symmetry of the action (but not necessarily the Lagrangian) under time reparametrizations.\([32,33,34,35]\) Invariance of the action leads to the selection of the SO(2,1) conformal group, as for the inverse square potential\([33]\), the magnetic monopole\([34]\), and the magnetic vortex.\([35]\) The corresponding generators are:

(i) the Hamiltonian \( H \), associated with time translations \( t \rightarrow t - \alpha \);
(ii) the dilation generator

\[
D = tH - \frac{1}{4}(r \cdot p + p \cdot r),
\]

(26)
associated with a scale transformation \( t \to \tau t; \mathbf{r} \to \tau^{1/2} \mathbf{r} \);

(iii) the special conformal generator

\[
K = H t^2 - \frac{1}{2} (\mathbf{p} \cdot \mathbf{r} + \mathbf{r} \cdot \mathbf{p}) t + \frac{1}{2} m v^2 ,
\]

(27)

associated with the special conformal transformation with respect to time \( 1/t \to 1/t + \alpha \).

These three generators satisfy the commutator relations: \([D, H] = -i \hbar H, [D, K] = i \hbar K,\) and \([H, K] = 2i \hbar D,\) which show that they form an SO(2,1) algebra. The same algebra is displayed by the two-dimensional delta-function interaction.\[10,18\]

The anomalous version of this algebra as a consequence of the breakdown of the classical SO(2,1) symmetry is currently being investigated and will be reported elsewhere.

This quantum symmetry breaking of SO(2,1) invariance is exhibited in Nature at the level of molecular physics, where it is realized in the point-dipole approximation.\[23\]

In particular, the interaction between an electron and a polar molecule can be reduced to a radial problem with an inverse square potential, for which the analysis of this paper applies. This information is then transferred to the angular part of the problem, which provides a critical dipole moment for electron capture and formation of anions—a result of unusual relevance and which is confirmed by a large body of existing experimental and numerical evidence.\[36,37\] This is indeed the most remarkable example of a quantum anomaly.\[23\]

In summary, we have completed a derivation of the energy Green’s function for the regularized inverse square potential (using a regularization “à la” field theory) in the (strong) supercritical regime. This problem provides an example illustrating that the use of intrinsically nonperturbative techniques (operator Green’s function approach) yields results identical to the corresponding ones derived from the infinite summation of perturbation theory to all orders.

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