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Green function for an axially symmetric potential field: a path integral evaluation in polar coordinates

M Victoria Carpio-Bernido

National Institute of Physics, University of the Philippines, Diliman, Quezon City 1101, The Philippines

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Abstract. An explicit evaluation of the path integral in spherical polar coordinates for the Green function of a particle moving in an axially symmetric potential field is presented. A closed form of the Green function is obtained from which the energy eigenvalues and the normalized eigenfunctions are obtained as the poles and the residues at the poles, respectively.

1. Introduction

Through a path integral derivation of the Green function, the exact wavefunctions and energy spectrum will be obtained for a non-relativistic particle of mass M moving in the three-dimensional axially symmetric potential field described by

$$V(\mathbf{r}) = \eta \sigma^2 \left\{ \frac{2a_0}{r} - q\eta \frac{a_0^2}{r^2 \sin^2 \theta} - g\eta \frac{a_0^2 \cos \theta}{r^2 \sin^2 \theta} \right\} \varepsilon_0$$
(1.1)

where $a_0 = (\hbar^2/Me^2)$ and $\varepsilon_0 = (-Me^4/2\hbar^2)$ are the Bohr radius and the ground-state energy of the hydrogen atom, respectively. η and σ are positive dimensionless parameters that can be adjusted to regulate the potential minimum while q and g are constants such that $q \ge |g|$. As seen from (1.1), the particle is constrained to move in the torus-shaped potential field with the entire z-axis ($\theta = 0, \pi$) as an inaccessible region. When q = 1 and g = 0, V reduces to the Hartmann potential [1]. When $g = \pm q$, we have $V \propto \{q/r^2(1 \mp \cos \theta)\}$, which have line singularities on the $\theta = 0$ or $\theta = \pi$ half-lines. The case q = g = 0 corresponds to the Coulomb potential.

The potential V belongs to a class of potentials included in the systematic search by Makarov *et al* [2] for systems with dynamical symmetries for which they found extra integrals of motion. Although the special case of the Hartmann potential has been the subject of interest in recent years [3-8], the possibility of working with the more general potential in the form (1.1) as a physically applicable model for axially symmetric systems remains to be investigated. Interestingly, the solutions for the special cases $g = \pm q$ remind us of the monopole harmonics of Wu and Yang [9], the spinweighted spherical harmonics of Newman and Penrose [10] and those of the symmetric top [11]. The connection between these functions are discussed in [12].

Using Feynman's path integral approach, the Green function will be derived *directly* in spherical polar coordinates by applying the techniques in polar coordinate path integration [13, 14] and the procedure for handling the Coulomb-type radial path

integral [15]. With this method, a closed form for the Green function is obtained in terms of Whittaker functions of the radial variable, hypergeometric functions of the polar angle θ , and the usual azimuthal dependence for axially symmetric systems. The negative energy eigenvalues are obtained from the poles of the Green function and the residues at the poles provide the correctly normalized wavefunctions. Our results coincide with those derived earlier using the path integral approach [16] but which involved the application of the Kustaanheimo-Stiefel (KS) transformation of coordinates and reparametrization of time [17]. The KS procedure has been used to reduce the path integral for the Coulomb-Green function into harmonic oscillator form [18, 19]. However, since the KS transformation is a non-bijective transformation which converts the problem for V in R^3 into that of two two-dimensional harmonic-plusinverse-square oscillators in R^4 subject to a constraint, its application within the path integral is highly non-trivial. Thus, the evaluation of the path integral for the Green function directly in spherical polar coordinates provides a more natural and straightforward alternative to our earlier path integral treatment using the KS transformation.

2. Path integral derivation of the Green function

In Feynman's formulation, the propagator is given as the path integral [20],

$$K(\mathbf{r}'',\mathbf{r}';\tau) = \int \exp[(i/\hbar)S]\mathscr{D}\mathbf{r}(t)$$
(2.1)

where $\mathfrak{D}\mathbf{r}(t)$ indicates an integration over all paths linking \mathbf{r}' and \mathbf{r}'' , and $S = \int_{t'}^{t''} L \, dt$. For systems with Coulomb-type radial dependence, the propagator has not been found in closed form. Hence, the Green function $G(\mathbf{r}'', \mathbf{r}'; E) = \langle \mathbf{r}'' | (E - H)^{-1} | \mathbf{r}' \rangle$ is evaluated instead since its poles and residues at the poles yield the energy spectrum and the wavefunctions. To accommodate the explicit calculation of the Green function within the path integral method, we note that the Fourier transform of the propagator gives

$$G(\mathbf{r}'', \mathbf{r}'; E) = (i\hbar)^{-1} \int K(\mathbf{r}'', \mathbf{r}'; \tau) \exp(iE\tau/\hbar) d\tau \qquad (2.2)$$

which can be rewritten as

$$G(\mathbf{r}'',\mathbf{r}';E) = (i\hbar)^{-1} \int P(\mathbf{r}'',\mathbf{r}';\tau) \,\mathrm{d}\tau$$
(2.3)

where $\tau = t'' - t'$ and $P(\mathbf{r}'', \mathbf{r}'; \tau) = \langle \mathbf{r}'' | \exp\{-(i/\hbar)\tau(H-E)\} | \mathbf{r}' \rangle$. In view of the role it plays in the application of coordinate-dependent time transformations in the path integral, $P(\mathbf{r}'', \mathbf{r}'; \tau)$ has been called the promotor [21]. It can be expressed as a path integral analogous to (2.1) but given in terms of the modified action (Hamilton's characteristic function), $W = \int (L+E) dt$. In time-sliced form, the promotor is given by

$$P(\mathbf{r}'', \mathbf{r}'; \tau) = \lim_{N \to \infty} \int \prod_{j=1}^{N} \exp[(i/\hbar) W_j] \prod_{j=1}^{N} [M/2\pi i \hbar \tau_j]^{3/2} \prod_{j=1}^{N-1} d\mathbf{r}_j. \quad (2.4)$$

Here, $(\tau/N) = \tau_j = t_j - t_{j-1}$, $r_j = r(t_j)$, $r_0 = r'$, $r_N = r''$, and the modified action for each short-time interval is

$$W_j = (M/2\tau_j)(\Delta r_j)^2 - V(r_j)\tau_j + E\tau_j.$$
(2.5)

In spherical polar coordinates, $r \in (0, \infty)$, $\theta \in (0, \pi)$ and $\phi \in (0, 2\pi)$, determined by the relations, $x = r \sin \theta \cos \phi$, $y = r \sin \theta \sin \phi$, and $z = r \cos \theta$, the short-time modified action for the system described by an axially symmetric potential takes the form:

$$W_{j} = (M/2\tau_{j})\{r_{j}^{2} + r_{j-1}^{2} - 2r_{j}r_{j-1}\cos\theta_{j}\cos\theta_{j-1} - 2r_{j}r_{j-1}\sin\theta_{j}\sin\theta_{j-1} \\ \times \cos(\phi_{j} - \phi_{j-1})\} - V(r_{j}, \theta_{j})\tau_{j} + E\tau_{j}.$$
(2.6)

The corresponding measure of the path integral in (2.4) is

$$\prod_{j=1}^{N} (M/2\pi i\hbar\tau_j)^{3/2} \prod_{j=1}^{N-1} d^3 \mathbf{r}_j = \prod_{j=1}^{N} (M/2\pi i\hbar\tau_j)^{3/2} \prod_{j=1}^{N-1} r_j^2 \sin\theta_j \, dr_j \, d\theta_j \, d\phi_j.$$
(2.7)

By making use of the expansion,

$$\exp(\xi\cos\delta/\tau_j) = \sum_{m=-\infty}^{\infty} \exp(im\delta)I_m(\xi/\tau_j)$$
(2.8)

the ϕ -dependent terms can immediately be separated allowing us to write:

$$\exp(iW_{j}/\hbar) = \sum_{m=-\infty}^{\infty} \exp\{im(\Delta\phi_{j})\} \exp[(iM/2\hbar\tau_{j})\{r_{j}^{2} + r_{j-1}^{2} - 2r_{j}r_{j-1}\cos\theta_{j}\cos\theta_{j-1}\}]$$

$$\times I_m(Mr_jr_{j-1}\sin\theta_j\sin\theta_{j-1}/i\hbar\tau_j)\exp\{i\tau_j E/\hbar - i\tau_j V(r_j,\theta_j)/\hbar\}.$$
 (2.9)

In turn, the modified Bessel function $I_{\lambda}(\xi/\tau_i)$ in (2.8) can be expanded for small τ_i as,

$$I_{\lambda}(\xi/\tau_j) \simeq (\tau_j/2\pi\xi)^{1/2} \exp\{(\xi/\tau_j) - \frac{1}{2}(\lambda^2 - \frac{1}{4})\tau_j/\xi + O(\tau_j^2)\}$$
(2.10)

where, for non-integral order λ , the modulus $|\lambda|$ is taken. Furthermore, in path integration, only terms up to first order in τ_j give significant contributions to the path integral. With (2.10), we can express (2.9) in the form,

$$\exp(\mathrm{i} W_j/\hbar) = (\mathrm{i} \hbar \tau_j/2\pi M r_j r_{j-1} \sin \theta_j \sin \theta_{j-1})^{1/2} \sum_{m=-\infty}^{\infty} \exp\{\mathrm{i} m(\Delta \phi_j)\}$$
$$\times \exp[(\mathrm{i} M/2\hbar \tau_j)(r_j^2 + r_{j-1}^2) + (M/\mathrm{i} \hbar \tau_j)r_j r_{j-1} \cos(\Delta \theta_j)$$
$$-\frac{1}{2}(m^2 - \frac{1}{4})\mathrm{i} \hbar \tau_j/M r_j r_{j-1} \sin \theta_j \sin \theta_{j-1} - \mathrm{i} \tau_j V(r_j, \theta_j)/\hbar + \mathrm{i} \tau_j E/\hbar\}.$$
(2.11)

Then, we notice that, if in (1.1) we make the substitutions, $A = -(q+g)\eta^2 \sigma^2 a_0^2 \varepsilon_0$, $B = -(q-g)\eta^2 \sigma^2 a_0^2 \varepsilon_0$, and $\kappa = -2\eta \sigma^2 a_0 \varepsilon_0$, we get

$$V(r_{j}, \theta_{j}) = -\frac{\kappa}{r_{j}} + \frac{A}{4r_{j}r_{j-1}\sin(\frac{1}{2}\theta_{j})\sin(\frac{1}{2}\theta_{j-1})} + \frac{B}{4r_{j}r_{j-1}\cos(\frac{1}{2}\theta_{j})\cos(\frac{1}{2}\theta_{j-1})}.$$
 (2.12)

The angular kinetic term can also be expressed in terms of half-angles as

$$\exp\{(M/i\hbar\tau_j)r_jr_{j-1}\cos(\Delta\theta_j)\}$$

=
$$\exp\{4Mr_jr_{j-1}\cos(\frac{1}{2}\Delta\theta_j)/i\hbar\tau_j + (3i\hbar\tau_j/32Mr_jr_{j-1})$$

$$-3Mr_jr_{j-1}/i\hbar\tau_j + O(\tau_j^2)\}$$
(2.13)

where we have used the relation

$$\cos(\Delta\theta_j) = 4\cos(\frac{1}{2}\Delta\theta_j) - 3 + \frac{1}{2}(\frac{1}{2}\Delta\theta_j)^4 + O(\tau_j^2).$$

The fourth-order terms have been replaced,

$$\exp\{(Mr_jr_{j-1}/2i\hbar\tau_j)(\frac{1}{2}\Delta\theta_j)^4\} \to \exp(3i\hbar\tau_j/32Mr_jr_{j-1})$$
(2.14)

following the procedure in appendix A of [14]. Thus, with (2.12) and (2.13), we arrive at the relation,

$$\exp(iW_{j}/\hbar) = (i\hbar\tau_{j}/8\pi Mr_{j}r_{j-1})^{1/2} \{\sin(\frac{1}{2}\theta_{j}) \sin(\frac{1}{2}\theta_{j-1})\}^{1/2} \{\cos(\frac{1}{2}\theta_{j}) \cos(\frac{1}{2}\theta_{j-1})\}^{-1/2} \\ \times \sum_{m=-\infty}^{\infty} \exp\{im(\Delta\phi_{j})\} \exp[(iM/2\hbar\tau_{j})(r_{j}^{2}+r_{j-1}^{2})+i\kappa\tau_{j}/\hbar r_{j}-3Mr_{j}r_{j-1}/i\hbar\tau_{j} \\ + 3i\hbar\tau_{j}/32Mr_{j}r_{j-1}+(4M/i\hbar\tau_{j})r_{j}r_{j-1}\cos(\frac{1}{2}\theta_{j})\cos(\frac{1}{2}\theta_{j-1}) \\ + (4M/i\hbar\tau_{j})r_{j}r_{j-1}\sin(\frac{1}{2}\theta_{j})\sin(\frac{1}{2}\theta_{j-1})+i\tau_{j}E/\hbar \\ - \{\frac{1}{2}(m^{2}-\frac{1}{4})+AM/\hbar^{2}\}\tau_{j}/(4M/i\hbar)r_{j}r_{j-1}\cos(\frac{1}{2}\theta_{j})\cos(\frac{1}{2}\theta_{j-1})] \\ - \{\frac{1}{2}(m^{2}-\frac{1}{4})+BM/\hbar^{2}\}\tau_{j}/(4M/i\hbar)r_{j}r_{j-1}\cos(\frac{1}{2}\theta_{j})\cos(\frac{1}{2}\theta_{j-1})]$$
(2.15)

which can be simplified by applying (2.10) once more. Equation (2.15) can then be rewritten as

$$\exp(iW_{j}/\hbar) = (\pi i\hbar\tau_{j}/2Mr_{j}r_{j-1})^{-1/2} \sum_{m=-\infty}^{\infty} \exp\{im(\Delta\phi_{j}) + (iM/2\hbar\tau_{j})(r_{j}^{2} + r_{j+1}^{2}) + i\kappa\tau_{j}/\hbar r_{j}\} \exp(i\tau_{j}E/\hbar) \exp(-\frac{3}{4}\zeta + 3/8\zeta) \times I_{\nu}\{\zeta \sin(\frac{1}{2}\theta_{j}) \sin(\frac{1}{2}\theta_{j-1})\} I_{\mu}\{\zeta \cos(\frac{1}{2}\theta_{j}) \cos(\frac{1}{2}\theta_{j-1})\}$$
(2.16)

where $\zeta = 4Mr_jr_{j-1}/i\hbar\tau_j$, $\nu = +(m^2 + 2AM/\hbar^2)^{1/2}$ and $\mu = +(m^2 + 2BM/\hbar^2)^{1/2}$. With (2.16), the terms depending on the polar angle can be separated from the radial ones by using the formula [22],

 $\zeta I_{\nu}(\zeta \sin \alpha \sin \beta) I_{\mu}(\zeta \cos \alpha \cos \beta) = 2(\sin \alpha \sin \beta)^{\nu} (\cos \alpha \cos \beta)^{\mu}$

$$\times \sum_{l=0}^{\infty} (\nu + \mu + 2l + 1) \Gamma(\nu + \mu + l + 1) \Gamma(\nu + l + 1)$$

$$\times \{l! \Gamma(\mu + l + 1)\}^{-1} \{\Gamma(\nu + 1)\}^{-2} I_{\nu + \mu + 2l + 1}(\zeta)$$

$$\times {}_{2}F_{1} \{-l, \nu + \mu + l + 1; \nu + 1; \sin^{2}(\frac{1}{2}\alpha)\}$$

$$\times {}_{2}F_{1} \{-l, \nu + \mu + l + 1; \nu + 1; \sin^{2}(\frac{1}{2}\beta)\}.$$

$$(2.17)$$

Using (2.17) in (2.16) and substituting the result in (2.4), we obtain the following expression involving the integrations of the angular terms

$$\sum_{m_{1},m_{2},...,m_{N}} \sum_{l_{1},l_{2},...,l_{N}} \int \prod_{j=1}^{N} \exp\{im_{j}(\phi_{j}-\phi_{j-1})\} \prod_{j=1}^{N} (\mu_{j}+\nu_{j}+2l_{j}+1)\mathcal{M}_{l_{j}} \\ \times {}_{2}F_{1}[-l_{j},\nu_{j}+\mu_{j}+l_{j}+1;\nu_{j}+1;\sin^{2}(\frac{1}{2}\theta_{j})] \\ \times {}_{2}F_{1}[-l_{1},\nu_{j}+\mu_{j}+l_{j}+1;\nu_{j}+1;\sin^{2}(\frac{1}{2}\theta_{j-1})] \\ \times \prod_{j=1}^{N-1} \sin \theta_{j} d\theta_{j} d\phi_{j}$$
(2.18)

where

$$\mathcal{M}_{l_j} = \frac{\Gamma(\nu_j + \mu_j + l_j + 1)\Gamma(\nu_j + \mu_j + 1)}{l_j!\Gamma(\mu_j + l_j + 1)\{\Gamma(\nu_j + 1)\}^2}$$

and with the summations and products interchanged. To perform the multiple integrations in (2.18), we use the orthonormalization for the hypergeometric polynomials [22],

$$\int_{0}^{\pi} \sin^{2\alpha}(\frac{1}{2}\theta) \cos^{2\beta}(\frac{1}{2}\theta) P_{\gamma}^{\alpha,\beta}(\cos\theta) P_{\rho}^{\alpha,\beta}(\cos\theta) \sin\theta \,d\theta$$
$$\cdot = \frac{2\Gamma(\gamma+\alpha+1)\Gamma(\gamma+\beta+1)}{(2\gamma+\alpha+\beta+1)\gamma!\Gamma(\gamma+\alpha+\beta+1)} \,\delta_{\gamma,\rho}$$
(2.19)

where the Jacobi polynomials are related to the hypergeometric functions as

$$P_{\gamma}^{\alpha,\beta}(x) = \binom{\gamma+\alpha}{\gamma}{}_{2}F_{1}(-\gamma,\gamma+\alpha+\beta+1;\alpha+1;\frac{1}{2}-\frac{1}{2}x).$$

Integration then yields the separated promotor for the axially symmetric potential V in (1.1):

$$P(r'', \theta'', \phi''; r', \theta, \phi'; \tau)$$

$$= (2\pi)^{-1} \sum_{m=-\infty}^{\infty} \sum_{l=0}^{\infty} \exp\{im(\phi'' - \phi')\}$$

$$\times (\nu + \mu + 2l + 1)[\Gamma(\nu + \mu + l + 1)\Gamma(\nu + l + 1)/l!\Gamma(\mu + l + 1)\{\Gamma(\nu + 1)\}^{2}]$$

$$\times {}_{2}F_{1}\{-l, \nu + \mu + l + 1; \nu + 1; \sin^{2}(\frac{1}{2}\theta'')\}$$

$$\times {}_{2}F_{1}\{-l, \nu + \mu + l + 1; \nu + 1; \sin^{2}(\frac{1}{2}\theta')\}$$

$$\times {}_{2}\cos(\frac{1}{2}\theta'')\cos(\frac{1}{2}\theta')\}^{\mu}\{\sin(\frac{1}{2}\theta'')\sin(\frac{1}{2}\theta')\}^{\nu}Q_{lm}(r'', r'; \tau) \qquad (2.20)$$

where the radial part is

 $Q_{lm}(r'',r';\tau)$

$$= \lim_{N \to \infty} (4\pi)^N \int \prod_{j=1}^N (\pi i \hbar \tau_j / 2Mr_j r_{j-1})^{1/2} \\ \times \exp[(iM/2\hbar \tau_j)(r_j^2 + r_{j-1}^2) + i\kappa \tau_j / \hbar r_j + iE\tau_j / \hbar] \\ \times I_{\frac{1}{2}(\nu+\mu)+l+\frac{1}{2}}(Mr_j r_{j-1} / i\hbar \tau_j) \prod_{j=1}^N (M/2\pi i\hbar \tau_j)^{3/2} \prod_{j=1}^{N-1} r_j^2 dr_j$$
(2.21)

which can be rewritten as

$$Q_{lm}(r'', r'; \tau) = (r''r')^{-1} \lim_{N \to \infty} \int \prod_{j=1}^{N} \exp[(iM/2\hbar\tau_j)(\Delta r_j)^2 + i\kappa\tau_j/\hbar r_j + iE\tau_j/\hbar - l'(l'+1)i\hbar\tau_j/2Mr_jr_{j-1}] \prod_{j=1}^{N} (M/2\pi i\hbar\tau_j) \prod_{j=1}^{N-1} dr_j$$
(2.22)

where $l' = \frac{1}{2}(\nu + \mu) + l$. The radial path integration for the promotor of the Coulomb potential as in (2.22) has been done by Inomata [15]. Using the result and performing the integration over τ in (2.3), we get the radial Green function,

$$G_{l'm}(r'', r'; E) = (M/i\hbar^2k)[(r''r')\Gamma(\nu+\mu+2l+2)]^{-1}\Gamma\{p+\frac{1}{2}(\nu+\mu)+l+1\} \times M_{-p,\frac{1}{2}(\nu+\mu)+l+\frac{1}{2}}(-2ikr')W_{-p,\frac{1}{2}(\nu+\mu)+l+\frac{1}{2}}(-2ikr'')$$
(2.23)

where $p = (-\kappa^2 M/2\hbar^2 E)^{1/2}$, $k = (2ME/\hbar^2)^{1/2}$, and M(x) and W(y) are the Whittaker functions.

3. Energy eigenvalues and eigenfunctions

The poles of the Green function yield the discrete energy spectrum. From (2.23), the simple poles correspond to $p + \frac{1}{2}(\nu + \mu) + l + l = -n_r$ for $n_r = 0, 1, 2, ...$, thus giving the energy eigenvalues:

$$E_{n_r,l,m} = \eta^2 \sigma^4 \varepsilon_0 / \{n_r + \frac{1}{2}(\nu + \mu) + l + 1\}^{-2}.$$
(3.1)

Note that for fixed m and $N = n_r + \frac{1}{2}(\nu + \mu) + l + 1$, there are degeneracies corresponding to combinations of n_r and l.

The radial wavefunctions can be obtained by evaluating the residues at the poles in the E-plane. This results in

$$R_{Nl}(r) = (M\kappa/\hbar^2 N^2)^{1/2} [r(\nu+\mu+2l+1)!]^{-1} \\ \times \{\Gamma[N+\frac{1}{2}(\nu+\mu)+l+1]/\Gamma[N-\frac{1}{2}(\nu+\mu)-l]\}^{1/2} \\ \times M_{N\lambda}(\nu+\mu)+l+\lambda} (2M\kappa r/\hbar^2 N)$$
(3.2)

or, in terms of the confluent hypergeometric functions,

$$R_{Nl}(r) = 2(M\kappa/\hbar^2)^{3/2}(2M\kappa r/\hbar^2)^l \exp(-M\kappa r/\hbar^2 N)\{n^{l+2}(\nu+\mu+2l+1)!\}^{-1} \\ \times [\Gamma\{N+\frac{1}{2}(\nu+\mu)+l+1\}/\Gamma\{N-\frac{1}{2}(\nu+\mu)-l\}]^{1/2} \\ \times {}_1F_1\{-N+\frac{1}{2}(\nu+\mu)+l+1, \nu+\mu+2l+1; 2M\kappa r/\hbar^2 N\}.$$
(3.3)

The angular wavefunctions can be obtained by inspection from (2.20). We have

$$\Phi_m(\phi) = (2\pi)^{-1/2} \exp(im\phi)$$
(3.4)

and

$$\Theta_{lm}(\theta) = [(\nu + \mu + 2l + 1)\Gamma(\nu + \mu + l + 1)\Gamma(\nu + l + 1)/l!\Gamma(\mu + l + 1)\{\Gamma(\nu + 1)\}^2]^{1/2} \\ \times \cos^{\mu}(\frac{1}{2}\theta)\sin^{\nu}(\frac{1}{2}\theta) {}_{2}F_{1}\{-l, \nu + \mu + l + 1; \nu + 1; \sin^{2}(\frac{1}{2}\theta)\}.$$
(3.5)

4. Conclusion

We have explicitly evaluated the path integral in spherical polar coordinates for the Green function of a particle moving in an axially symmetric potential field. The energy eigenvalues and normalized eigenfunctions were obtained as the poles and the residues at the poles of the Green function, respectively. Our results coincide with those of an earlier path integral treatment [16] involving the Kustaanheimo-Stiefel (κ s) transformation [17].

The procedure followed in this work has also been applied to charge-dyon systems [23].

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