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The Mehler formula and the Green function of the multi-dimensional isotropic harmonic oscillator†

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Abstract. Using a generalized Mehler formula, a closed representation is obtained for the Green function of the stationary Schrödinger equation for a multidimensional isotropic harmonic oscillator.

1. Derivation of the Green function

The present note contains a simple derivation of the Green function of the N dimensional harmonic oscillator using the generating function of the product of the harmonic oscillator wavefunction given by a generalized Mehler formula (Erdélyi 1953).

We define the Green function of the stationary Schrödinger equation for an N dimensional harmonic oscillator by means of the spectral decomposition

$$G^N(\mathbf{r}, \mathbf{r}', \lambda) = \sum_{\nu=0}^{\infty} (E_{\nu} - \lambda)^{-1} \sum_{\nu_1 + \nu_2 + \dots + \nu_N = \nu} \psi_{\nu_1}(x_1) \psi_{\nu_1}(x'_1) \dots \psi_{\nu_N}(x_N) \psi_{\nu_N}(x'_N) \quad (1)$$

where $\psi_{\nu_i}(x_i)$ is the harmonic oscillator wavefunction; $E_{\nu} = \nu + \frac{1}{2}N$ is the energy and \mathbf{r} is a radius vector in the N dimensional space. (We put $\hbar = m = \omega = 1$.)

The generalized Mehler formula for the N dimensional harmonic oscillator can be written in the following way (see appendix)

$$\begin{aligned} \pi^{N/2} \sum_{\nu=0}^{\infty} \xi^{\nu} \sum_{\nu_1 + \nu_2 + \dots + \nu_N = \nu} \psi_{\nu_1}(x_1) \psi_{\nu_1}(x'_1) \dots \psi_{\nu_N}(x_N) \psi_{\nu_N}(x'_N) \\ = (1 - \xi^2)^{-N/2} \exp\left[-\frac{1}{2}(\mathbf{r}^2 + \mathbf{r}'^2)\right] \exp\left(\frac{2\mathbf{r} \cdot \mathbf{r}' \xi - (\mathbf{r}^2 + \mathbf{r}'^2) \xi^2}{1 - \xi^2}\right). \end{aligned} \quad (2)$$

We see that the Mehler formula contains explicitly the full SU_N symmetry of the N dimensional harmonic oscillator.

We consider first the density matrix

$$\rho_r^N(\mathbf{r}, \mathbf{r}') = \text{res } G(\mathbf{r}, \mathbf{r}', E_{\nu}) = \sum_{\nu_1 + \nu_2 + \dots + \nu_N = \nu} \psi_{\nu_1}(x_1) \psi_{\nu_1}(x'_1) \dots \psi_{\nu_N}(x_N) \psi_{\nu_N}(x'_N). \quad (3)$$

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Using equation (2) we have

$$\rho_\nu^N(\mathbf{r}, \mathbf{r}') = \pi^{-N/2} \exp[-\frac{1}{2}(\mathbf{r}^2 + \mathbf{r}'^2)] \frac{1}{2\pi i} \oint_{\xi=0} d\xi \xi^{-(E_\nu - \frac{1}{2}N+1)} (1 - \xi^2)^{-N/2} \\ \times \exp\left(\frac{2\mathbf{r} \cdot \mathbf{r}' \xi - (\mathbf{r}^2 + \mathbf{r}'^2) \xi^2}{1 - \xi^2}\right). \quad (4)$$

The Green function is given by

$$G^N(\mathbf{r}, \mathbf{r}', \lambda) = \sum_{\nu=0}^{\infty} \frac{\rho_\nu^N(\mathbf{r}, \mathbf{r}')}{E_\nu - \lambda} \quad (5)$$

and for $\text{Re}(\frac{1}{2}N - \lambda) > 0$ can be cast into the form

$$G^N(\mathbf{r}, \mathbf{r}', \lambda) = \pi^{-N/2} \exp[-\frac{1}{2}(\mathbf{r}^2 + \mathbf{r}'^2)] \int_0^1 d\xi \xi^{(N/2), \lambda-1} \\ \times (1 - \xi^2)^{-N/2} \exp\left(\frac{2\mathbf{r} \cdot \mathbf{r}' \xi - (\mathbf{r}^2 + \mathbf{r}'^2) \xi^2}{1 - \xi^2}\right). \quad (6)$$

This integral representation is exactly the expression of Berendt and Weimar (1972) obtained using the full SU_N symmetry of the N dimensional harmonic oscillator in a Fock space representation. The singularities exhibited by equation (6) are the well known singularities of the harmonic oscillator Green function: none for $N=1$, a logarithmic one in the variable $|\mathbf{r} - \mathbf{r}'|$ for $N=2$ and a pole of order $N-2$ for higher N in that variable. A very simple variable transformation can also reproduce the results obtained by Bakhrakh *et al* (1972).

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Appendix

To prove equation (2) we start with the bilinear generating function of one N dimensional Hermite polynomial (Erdélyi 1953)

$$\sum \frac{t_1^{\nu_1} \dots t_N^{\nu_N}}{\nu_1! \dots \nu_N!} H_{\nu}(\mathbf{r}) H_{\nu}(\mathbf{r}') = (t_1 \dots t_N)^{-1} (\Delta_1 \Delta_2)^{-1/2} \exp[\frac{1}{4}\psi_1(C\mathbf{r} + C\mathbf{r}') - \frac{1}{4}\psi_2(C\mathbf{r} - C\mathbf{r}')] \quad (A.1)$$

with the following notation:

$$\phi(\mathbf{r}) = \sum_{i,j=1}^N C_{ij} x_i x_j \quad (A.2)$$

where C will be a fixed positive definite symmetric square matrix of real elements;

$$\begin{aligned}\phi_1(\mathbf{r}) &= \sum_{j=1}^N (x_j^2/t_j) + \phi(\mathbf{r}) \\ \phi_2(\mathbf{r}) &= \sum_{j=1}^N (x_j^2/t_j) - \phi(\mathbf{r})\end{aligned}\tag{A.3}$$

Δ_k is the determinant of ϕ_k , $k = 1, 2$. $\psi_k(\mathbf{r})$ is the reciprocal quadratic form of $\phi_k(\mathbf{r})$. For sufficiently small positive t_i , ϕ_k are positive definite.

If we put $t_1 = t_2 = \dots = t_N = \xi/2$ and $C_{ij} = 2\delta_{ij}$ we have for ϕ_k and ψ_k

$$\begin{aligned}\phi_1(\mathbf{r}) &= \sum_{i,j=1}^N (D_1)_{ij} x_i x_j; & \psi_1(\mathbf{r}) &= \sum_{i,j=1}^N (D_1^{-1})_{ij} x_i x_j \\ \phi_2(\mathbf{r}) &= \sum_{i,j=1}^N (D_2)_{ij} x_i x_j; & \psi_2(\mathbf{r}) &= \sum_{i,j=1}^N (D_2^{-1})_{ij} x_i x_j\end{aligned}\tag{A.4}$$

where $(D_{1,2})_{ij} = 2(1 \pm \xi)\delta_{ij}/\xi$, and equation (A.1) can be transformed into

$$\sum \frac{(\xi/2)^\nu}{\nu_1! \dots \nu_N!} H_{\nu}(\mathbf{r}) H_{\nu}(\mathbf{r}') = (1 - \xi^2)^{-N/2} \exp\left(\frac{2\mathbf{r} \cdot \mathbf{r}' \xi - (\mathbf{r}^2 + \mathbf{r}'^2)\xi^2}{1 - \xi^2}\right).\tag{A.5}$$

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