Free-particle and harmonic-oscillator propagators in two and three dimensions

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(*Recebido: 21 de outubro de 2002*)

Abstract: *This contribution illustrates how to construct free-particle and harmonic-oscillator quantum-mechanical propagators in two and three dimensions in cartesian, and in circular and spherical coordinates, respectively, starting from the corresponding one-dimensional propagators in cartesian coordinates.*

Key words: *quantum-mechanical propagator, free particle, harmonic oscillator*

Resumo: *Esta contribuição ilustra como construir propagadores para partícula livre e oscilador harmônico em duas e três dimensões, em coordenadas cartesianas, polares e esféricas, partindo do propagador correspondente em uma dimensão em coordenada cartesiana.*

Palavras-chave: *propagador quântico, partícula livre, oscilador harmônico*

1 Introduction

The study of quantum-mechanical propagators, or Green functions, in most textbooks is restricted to one-dimensional systems, including closed analytical forms for the free particle and the harmonic oscillator [1]-[4]. This contribution illustrates how to construct the corresponding Green functions in two and three dimensions in cartesian, and in circular and spherical coordinates, respectively. The basis for such an extension is the separability of the Schrödinger equation and the consequent factorability of its eigenfunctions and Green functions in the different coordinates.

Green functions, $K(\vec{r},\vec{r}\,';t)$, determine the time evolution of the quantum system's wave function,

$$\psi(\vec{r},t) = \int_0^t d^N r' K(\vec{r},\vec{r}\,';t)\psi(\vec{r},0). \tag{1}$$

They satisfy the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}K(\vec{r},\vec{r}\,';t) = \left[-\frac{\hbar^2}{2\mu}\nabla^2 + v(\vec{r})\right]K(\vec{r},\vec{r}\,';t), \tag{2}$$

and the initial condition

$$K(\vec{r},\vec{r}\,';t=0) = \delta(\vec{r}-\vec{r}\,'). \tag{3}$$

Correspondingly, the Green function can be constructed as the linear superposition

$$K(\vec{r},\vec{r}\,';t) = \sum_{n=0}^{\infty}\psi_n^*(\vec{r}\,')\psi_n(\vec{r})e^{-iE_nt/\hbar} \tag{4}$$

of the orthonormal eigenfunctions $\psi_n(\vec{r})$, each one evolving harmonically in time with the frequency $E_n/\hbar$ determined by the corresponding energy eigenvalues of the quantum system. For $t = 0$, the initial condition of Eq. (3) is obviously satisfied because of the completeness, or closure, property of the eigenfunctions.

In particular, Eq. (4) for the one-dimensional free-particle and harmonic-oscillator propagators takes the respective forms [1]-[6]

$$\begin{aligned} K_{fp}(x,x';t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ik(x-x')}e^{-i\hbar k^2 t/2\mu} \\ &= \left(\frac{\mu}{2\pi i\hbar t}\right)^{1/2} e^{-\mu(x-x')^2/(2i\hbar t)}, \end{aligned} \tag{5}$$

and

$$\begin{aligned} K_{ho}(x,x';t) &= \left(\frac{\mu\omega}{\pi\hbar}\right)^{1/2}\sum_{n=0}^{\infty}\frac{H_n(\sqrt{\frac{\mu\omega}{\hbar}}x')H_n(\sqrt{\frac{\mu\omega}{\hbar}}x)}{2^n n!}e^{-\mu\omega(x'^2+x^2)/2\hbar}e^{-i(n+\frac{1}{2})\omega t} \\ &= \left(\frac{\mu\omega}{2\pi i\hbar\sin\omega t}\right)^{1/2} e^{-\mu\omega(x^2\cos\omega t-2xx'+x'^2\cos\omega t)/(2i\hbar\sin\omega t)}, \end{aligned} \tag{6}$$

where $H_n(z)$ are the Hermite polynomials.

The task of constructing the corresponding propagators in two and three dimensions is accomplished in the next section in two successive stages.The first one in cartesian coordinates is straightforward, and the second one involves the change to circular or spherical coordinates as well as the change to the corresponding eigenfunctions and energy eigenvalues. In Section 3 we discuss some points of didactic interest.

2 Construction of the quantum propagators in two and three dimensions

The extensions of Eqs. (5) and (6) to N-dimensions in cartesian coordinates, $x_1 = x, x_2 = y, x_3 = z$, are obtained by direct multiplication

$$\begin{aligned} K_{fp}(\{x_q\},\{x'_q\};t) &= \frac{1}{(2\pi)^N}\prod_{s=1}^{N}\int_{-\infty}^{\infty} dk_s e^{ik_s(x_s-x'_s)}e^{-i\hbar k_s^2 t/2\mu} \\ &= \left(\frac{\mu}{2\pi i\hbar t}\right)^{N/2}\prod_{s=1}^{N} e^{-\mu(x_s-x'_s)^2/(2i\hbar t)}, \end{aligned} \tag{7}$$

and

$$\begin{aligned} &K_{ho}(\{x_q\},\{x'_q\};t) = \\ &= \prod_{s=1}^{N}\left(\frac{\mu\omega_s}{\pi\hbar}\right)^{1/2}\sum_{n_s=0}^{\infty}\frac{1}{2^{n_s}n_s!}H_{n_s}\left(\sqrt{\frac{\mu\omega_s}{\hbar}}x'_s\right)H_{n_s}\left(\sqrt{\frac{\mu\omega_s}{\hbar}}x_s\right) \\ &\times e^{-\mu\omega_s(x'^2_s+x_s^2)/2\hbar}e^{-i(n_s+\frac{1}{2})\omega_s t} \\ &= \prod_{s=1}^{N}\left(\frac{\mu\omega_s}{2\pi i\hbar\sin\omega_s t}\right)^{1/2} e^{-\mu\omega_s(x_s^2\cos\omega_s t-2x_s x'_s+x'^2_s\cos\omega_s t)/(2i\hbar\sin\omega_s t)}. \end{aligned} \tag{8}$$

In Eq. (7) the product of the gaussian exponentials is equal to a single gaussian exponential with argument

$$\frac{-\mu}{2i\hbar t}\sum_{s=1}^{N}(x_s-x'_s)^2 = \frac{-\mu}{2i\hbar t}(\vec{r}-\vec{r}\,')^2.$$

The propagator of Eq. (8) is valid in general for anisotropic harmonic oscillators, *i. e.*, $\omega_x \neq \omega_y \neq \omega_z$; but, it can be simplified further for isotropic harmonic oscillators, *i. e.*, $\omega_x = \omega_y = \omega_z = \omega$, for which

$$\sum_{s=1}^{N} x_s^2 = r_s^2 \qquad \text{and} \qquad \sum_{s=1}^{N} x_s x'_s = \vec{r}_s\cdot\vec{r}\,'_s$$

in the product of the exponentials.

The adaptations of Eq. (4) and the changes of Eq. (7) to circular and spherical coordinates and the corresponding eigenfunctions and eigenvalues lead to the respective free-particle propagators in $N = 2$ and 3 dimensions:

$$\begin{aligned} K_{fp}(R,\varphi;R',\varphi';t) &= \sum_{m=-\infty}^{\infty}\int_0^{\infty} dk\,kJ_m(kR')J_m(kR)\frac{e^{im(\varphi-\varphi')}}{2\pi}e^{-i\hbar k^2 t/2\mu} \\ &= \left(\frac{\mu\omega}{2\pi i\hbar t}\right)e^{-\mu[R^2-2RR'\cos(\varphi-\varphi')+R'^2]/(2i\hbar t)}, \end{aligned} \tag{9}$$

and

$$
\begin{aligned}
K_{fp}(r,\theta,\varphi;r',\theta',\varphi';t) &= \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{2}{\pi}\int_0^{\infty} dk\, k^2 j_l(kr')j_l(kr) \\
&\quad \times Y^*_{lm}(\theta',\varphi')Y_{lm}(\theta,\varphi)e^{-i\hbar k^2 t/2\mu} \\
&= \left(\frac{\mu\omega}{2\pi i\hbar t}\right)^{3/2} e^{-\mu[r^2-2\vec{r}\cdot\vec{r}\,'+r'^2]/2i\hbar t}, \qquad (10)
\end{aligned}
$$

where $J_m(z)$ and $j_l(z)$ are the ordinary and spherical Bessel functions, respectively, and $Y_{lm}(\theta,\varphi)$ are the spherical harmonics. Likewise, the propagators for the isotropic harmonic oscillators in circular and spherical coordinates are constructed via Eqs. (4) and (8) with the results

$$
\begin{aligned}
& K_{ho}(R,\varphi;R',\varphi';t) \\
&= \left(\frac{\mu\omega}{\hbar}\right)\sum_{n=0}^{\infty}\sum_{m=-\infty}^{\infty}\frac{2(n!)}{(n+m)!}\left(\sqrt{\frac{\mu\omega}{\hbar}}R'\right)^{|m|} L_n^{(|m|)}\left(\frac{\mu\omega}{\hbar}R'^2\right) \\
&\times \left(\sqrt{\frac{\mu\omega}{\hbar}}R\right)^{|m|} L_n^{(|m|)}\left(\frac{\mu\omega}{\hbar}R^2\right) e^{-\mu\omega(R'^2+R^2)/2\hbar}\,\frac{e^{im(\varphi-\varphi')}}{2\pi}\, e^{-i(2n+|m|+1)\omega t} \\
&= \left(\frac{\mu\omega}{2\pi i\hbar\sin\omega t}\right) e^{-\mu\omega(R^2\cos\omega t-2\vec{R}\cdot\vec{R}'+R'^2\cos\omega t)/(2i\hbar\sin\omega t)}, \qquad (11)
\end{aligned}
$$

and

$$
\begin{aligned}
& K_{ho}(r,\theta,\varphi;r',\theta,\varphi';t) \\
&= \left(\frac{\mu\omega}{\hbar}\right)^{3/2}\sum_{n=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{2(n!)}{\Gamma(n+l+3/2)}\left(\sqrt{\frac{\mu\omega}{\hbar}}r'\right)^{l} L_n^{(l+\frac{1}{2})}\left(\frac{\mu\omega}{\hbar}r'^2\right) \\
&\times \left(\sqrt{\frac{\mu\omega}{\hbar}}r\right)^{l} L_n^{(l+\frac{1}{2})}\left(\frac{\mu\omega}{\hbar}r^2\right) e^{-\mu\omega(r'^2+r^2)/2\hbar} Y^*_{lm}(\theta',\varphi')Y_{lm}(\theta,\varphi)e^{-i(2n+l+3/2)\omega t} \\
&= \left(\frac{\mu\omega}{2\pi i\hbar\sin\omega t}\right)^{3/2} e^{-\mu\omega(r^2\cos\omega t-2\vec{r}\cdot\vec{r}\,'+r'^2\cos\omega t)/(2i\hbar\sin\omega t)}. \qquad (12)
\end{aligned}
$$

in terms of the circular and spherical radial Laguerre polynomials $L_n^{(\alpha)}(z)$ and angular harmonics, respectively.

This section can be concluded by recognizing that Eqs. (7) and (8) are the quantum propagators in N dimensions in cartesian coordinates for the free particle and harmonic oscillator, respectively. Correspondingly, the respective propagators for $N = 2$ in circular coordinates are given by Eqs. (9) and (11) and for $N = 3$ in spherical coordinates by Eqs. (10) and (12).

3 Discussion

The general construction of quantum propagators, Eq. (4), requires the solution of the Schrödinger Eq. (2) subject to the initial condition of Eq. (3). For the free particle and the harmonic oscillator in one dimension and cartesian coordinates the sumations of Eqs. (5) and (6) have been explicitly done [1]-[6]. The extension to higher dimensions in cartesian coordinates, Eqs. (7) and (8), are immediate for both quantum systems on account of the separability of the Schrödinger equation.

It is well known that the Schrödinger equation for both systems is also separable in circular and spherical coordinates for two and three dimensions, respectively. Consequently, the steps from Eqs. (7) to (9) and (10) correspond to the changes from cartesian coordinates and plane waves to circular and spherical coordinates and waves, respectively. Their study can be implemented after having learned about the free particle in states with well-defined angular momentum. Similar comments are valid for the steps from Eq. (8) to (11) and (12) for the harmonic oscillators.

Comparison of Eqs. (9)-(12) with Eq. (4) allows the identification of the orthonormal eigenfunctions $\psi_n(\vec{r})$ and eigenenergies for each system in the corresponding coordinates. The solution of Eq. (2) subject to the initial condition of Eq. (3) is the same in the different coordinate systems, guaranteeing by construction the validity of Eqs. (9)-(12). Of course, if the reader is interested in proving their validity independently of the context of this paper, the easiest way to do it is to expand the exponentials using the Rayleigh expansion for the angular dependent factor and resumming. Part of the didactic value of our results is the ease with which they can be obtained, understood and explained.

While Eqs. (7) and (8) are valid for any dimension N, the propagators of (9)-(12) have been written explicitly for $N = 2$ and 3. The extension to higher dimensions using hyperspherical coordinates and hyperspherical harmonics can also be implemented for both the free particle and the harmonic oscillator.

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