

CONSTRUCTION OF THE GREEN'S FUNCTION
FOR THE PSEUDOHARMONICAL OSCILLATOR

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In the present paper we have constructed the Green's function for the pseudoharmonic potential, which is considered as an intermediate potential between the harmonic and anharmonic potentials. We have used a hybrid method, by combining the Laplace transformation method and the Green's function technique. The Green's function is used for obtaining the density matrix for a quantum-statistical system, in coordinate representation. Even if this is not a new result, the method can be applied to a class of exactly solvable potentials.

1 Preliminaries

In the past years there has been a considerable interest for the pseudoharmonic oscillator (PHO) potential [1–3]:

$$V^{(p)}(r) = \frac{m\omega^2}{8}r_0^2 \left(\frac{r}{r_0} - \frac{r_0}{r} \right)^2, \quad (1)$$

when r_0 is the equilibrium position of the oscillator of mass m and frequency ω . Here and bellow, the index (p) refers to the characteristic quantities of PHO.

Particularly, it is of interest to construct the density matrix of PHO, via the Green's function, due to the fact that PHO admits an exact analytical solution of the Schrödinger equation. At the same time, by means of the harmonical limit ($r_0 \rightarrow 0$), the PHO passes to the harmonical three-dimensional (HO-3D) potential, which is a mathematically rigorously solvable problem. In this manner, the obtained results for the PHO can be easily verified by comparing with the corresponding results for the HO-3D. On the other hand, PHO is, in a certain sense, an intermediate potential between the harmonic three-dimensional oscillator potential (which is an ideal potential) and the anharmonic potentials, as the Morse oscillator (MO) potential, which is a more realistic potential, in good agreement with the experimental spectroscopical data.

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We consider the simplest quantum-mechanical system, namely, a spinless particle in the central potential (1). The motion of this system is governed by the Schrödinger equation, with the Hamiltonian:

$$H(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2 + V^{(p)}(r), \quad (2)$$

which can be transformed in the traditional manner as follows:

$$\left[-\frac{\hbar^2}{2m}\nabla_r^2 + V_J^{(p)}(r)\right] R_{vJ}^{(p)} = E_{vJ}^{(p)} R_{vJ}^{(p)}(r), \quad (3)$$

where v , J and M are the principal, the orbital and the magnetic quantum numbers, respectively, and $R_{vJ}^{(p)}(r)$ are the radial function of the eigenfunction $\Psi_{vJM}^{(p)}(\vec{r})$ of the Hamiltonian (2). The potential

$$V_J^{(p)}(r) = V^{(p)}(r) + \frac{\hbar^2}{2m} \frac{J(J+1)}{r^2} \quad (4)$$

is the effective potential. The interest towards effective potentials proceeds from the fact that these potentials, in different approximations, facilitate the obtaining of analytical results for the molecular wave functions and evaluating molecular vibration-rotation spectra. The most usual approximation method of the effective pseudoharmonic vibration-rotation potential is to rewrite it as a shifted pseudoharmonic potential with the same force constant as there for the corresponding centered ($r_0 = 0$) three-dimensional harmonic oscillator [2]. We propose a rather different way. By using an idea of Molski [4], the effective PHO potential can be easily transformed in the following manner:

$$V_J^{(p)}(r) = \frac{m\omega^2}{8} r_J^2 \left(\frac{r}{r_J} - \frac{r_J}{r}\right)^2 + E_{0J}^{(p)}, \quad (5)$$

$$E_{0J}^{(p)} = \frac{m\omega^2}{4} (r_J^2 - r_0^2), \quad (6)$$

$$r_J = r_0 \left[1 + \left(\frac{2\hbar}{m\omega r_0^2}\right)^2 J(J+1)\right]^{1/4}. \quad (7)$$

The oscillator with the potential (5) is called the displaced PHO (with $J \neq 0$). In comparison with the nondisplaced PHO (with $J = 0$), the displaced PHO has the same frequency ω and the same mass m , so that we can talk about the same oscillator. When we consider the rotation ($J \neq 0$), this fact has as a consequence the scale shift of the energy, so that Schrödinger's equation (3) becomes:

$$\left[-\frac{\hbar^2}{2m}\nabla_r^2 + \frac{m\omega^2}{8} r_J^2 \left(\frac{r}{r_J} - \frac{r_J}{r}\right)^2\right] R_{vJ}^{(p)}(r) = (E_{vJ}^{(p)} - E_{0J}^{(p)}) R_{vJ}^{(p)}(r) \equiv \varepsilon_{vJ} R_{vJ}^{(p)}(r). \quad (8)$$

In the right-hand side of this equation we can see that the energy $E_{vJ}^{(p)}$ is diminished by the quantity $E_{0J}^{(p)}$ (called the effective rotation energy). This fact is a consequence of the equilibrium position change $r_0 \rightarrow r_J$, caused by the centrifugal force.

Let us consider a system of identical pseudoharmonical oscillators (the quantum gas), without interactions, which are in thermodynamical equilibrium with the reservoir (thermostat) at temperature $T = (k_B \beta)^{-1}$. This system obeys the quantum canonical distribution, characterized by the canonical density matrix, which will be deduced by means of the Green's function.

In the coordinate (position) representation, the global density matrix may be expressed as follows [3]:

$$\rho^{(p)}(\vec{r}, \vec{r}'; \beta) = \frac{1}{4\pi} \sum_J (2J+1) P_J(\cos \gamma) \rho_J^{(p)}(r, r', \beta), \quad (9)$$

while the radial density matrix is

$$\rho_J^{(p)}(r, r'; \beta) = \sum_v \exp(-\beta E_{vJ}^{(p)}) R_{vJ}^{(p)}(r) R_{vJ}^{(p)*}(r'), \quad (10)$$

where we have used the orthogonality properties of the angular functions $Y_{JM}(\theta, \varphi)$. Here $P_J(\cos \gamma)$ is Legendre's polynomial, γ — the angle between the vectors $\vec{r}$ and $\vec{r}'$ and $R_{vJ}^{(p)}(r)$ — the radial part of the eigenfunction $\Psi_{vJM}^{(p)}(\vec{r})$.

The global density matrix (9) satisfies the Bloch equation

$$-\frac{\partial}{\partial \beta} \rho^{(p)}(\vec{r}, \vec{r}'; \beta) = H(\vec{r}) \rho^{(p)}(\vec{r}, \vec{r}'; \beta) \quad (11)$$

with the limiting condition

$$\lim_{\beta \rightarrow 0} \rho^{(p)}(\vec{r}, \vec{r}'; \beta) = \delta(\vec{r} - \vec{r}'), \quad (12)$$

where the 3D Dirac distribution is (see, e.g. [5]):

$$\delta(\vec{r} - \vec{r}') = \frac{1}{rr'} \delta(r - r') \frac{1}{\sin \theta} \delta(\theta - \theta') \delta(\varphi - \varphi'). \quad (13)$$

Generally speaking, for a Bloch equation involving the Hamiltonian $H(\vec{r})$ and the energy eigenvalue E , like Eqs. (11) and (12), a function $G(\vec{r}, \vec{r}'; E)$ defined as:

$$G(\vec{r}, \vec{r}'; E) = \int_0^\infty e^{-\beta E} \rho(\vec{r}, \vec{r}'; \beta) d\beta, \quad (14)$$

leads to the Green's equation for the Hamiltonian $H(\vec{r})$:

$$[H(\vec{r}) - E] G(\vec{r}, \vec{r}'; E) = \delta(\vec{r} - \vec{r}'). \quad (15)$$

Therefore, the density matrix in the coordinate (position) representation $\rho(\vec{r}, \vec{r}'; \beta)$ plays the role of the inverse Laplace transform of Green's function $G(\vec{r}, \vec{r}'; E)$ of the Hamiltonian $H(\vec{r})$, these two functions being related one to another. Then, the density matrix becomes:

$$\rho(\vec{r}, \vec{r}'; \beta) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} G(\vec{r}, \vec{r}'; E) e^{\beta E} dE = \sum_{n=1}^N \text{Res}_n [G(\vec{r}, \vec{r}'; E) e^{\beta E}]. \quad (16)$$

The canonical density operator ρ is the operator with the maximal significance for the quantum-statistical approach of any system which is in the state of the thermodynamical equilibrium with the reservoir (thermostat) [6]. Consequently, it is very important to know the density operator (or, in a certain representation, the density matrix) of the examined system, because the expected value of a certain physical observable, which characterizes the quantum system, is expressed through the density matrix.

In the case of the quantum system, which we have examined, i.e. the PHO-quantum gas, the expected value of such a physical observable $A^{(p)}$ is

$$\langle A^{(p)} \rangle = \frac{1}{Z^{(p)}(\beta)} \int A^{(p)}(\vec{r}') \rho^{(p)}(\vec{r}, \vec{r}'; \beta) \Big|_{\vec{r}'=\vec{r}} d\vec{r}, \quad (17)$$

where the trace of the density matrix is just the partition function $Z^{(p)}(\beta)$ and the succession of the operations is the following: first, the operator $A^{(p)}(\vec{r}')$ acts on the function $\rho(\vec{r}, \vec{r}'; \beta)$ (acting only on the dashed variable $\vec{r}'$), then the dash is deleted. Finally, integration is performed over the variables without the dash [7].

Because the PHO-potential (1) is a central field potential, the radial density matrix (10) also satisfies the Bloch equation

$$-\frac{\partial}{\partial \beta} \rho_j^{(p)}(r, r'; \beta) = \left[-\frac{\hbar^2}{2m} \nabla_r^2 + \frac{m\omega^2}{8} r_j^2 \left(\frac{r}{r_j} - \frac{r_j}{r} \right)^2 + E_{0j}^{(p)} \right] \rho_j^{(p)}(r, r'; \beta), \quad (18)$$

$$\lim_{\beta \rightarrow 0} \rho_j^{(p)}(r, r'; \beta) = \frac{1}{rr'} \delta(r - r'). \quad (19)$$

Similar with Ref. 3, we use the following function substitution:

$$g_j^{(p)}(r, r'; \beta) = rr' \rho_j^{(p)}(r, r'; \beta) \exp(\beta E_{0j}^{(p)}) \quad (20)$$

and the Bloch equation for this new function, which is called reduced density matrix, becomes:

$$-\frac{\partial}{\partial \beta} g_j^{(p)}(r, r'; \beta) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + \frac{m\omega^2}{8} r_j^2 \left(\frac{r}{r_j} - \frac{r_j}{r} \right)^2 \right] g_j^{(p)}(r, r'; \beta). \quad (21)$$

By means of these manipulations, we have obtained a Bloch equation similar to the Bloch equation for the nonrotating (one dimensional) PHO motion and of course, this case is easier to deal with.

2 Green's function

For solving Eq. (21) we adopt the Green's function method. At first, we introduce the Laplace's transform of reduced radial density matrix (20):

$$G_J^{(p)}(r, r'; s) = \mathcal{L} \left[g_J^{(p)}(r, r'; \beta) \right] \equiv \int_0^\infty e^{-s\beta} g_J^{(p)}(r, r'; \beta) d\beta. \quad (22)$$

So, by multiplying Eq. (21) by $\exp(-s\beta)$ and integrating over the variable $\beta = (k_B T)^{-1}$, where T is the equilibrium absolute temperature, due to the limiting condition (19), we obtain the following equation for the Green's function (22):

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{m\omega^2}{8} r_J^2 \left(\frac{r}{r_J} - \frac{r_J}{r} \right)^2 + s \right] G_J^{(p)}(r, r'; s) = \delta(r - r'), \quad (23)$$

where, see Eq. (8), $s \equiv -\varepsilon_{vJ} = -(E_{vJ}^{(p)} - E_{0J}^{(p)})$, i.e. the sign opposite eigenvalue of the Schrödinger equation (8) for the PHO.

By using the notation

$$\tilde{E} = \frac{1}{4} m\omega^2 r_J^2 - s = E_{vJ}^{(p)} + \frac{1}{4} m\omega^2 r_0^2, \quad (24)$$

this equation can be written again in the following appearance:

$$\left[-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} - \frac{2m}{\hbar^2} \frac{m\omega^2}{8} r_J^4 \frac{1}{r^2} \right) + \frac{m\omega^2}{8} r^2 - \tilde{E} \right] \tilde{G}_J(r, r'; \tilde{E}) = -i\hbar \delta(r - r'), \quad (25)$$

which is similar to Eqs. (3) and (5) of the paper of Chetouani et al. [8]. In this paper, the Green's function for the Morse potential is calculated in the SO(2,1) algebraic approach. In Eq. (25) we have used the new function:

$$\tilde{G}_J(r, r'; \tilde{E}) = -i\hbar G_J^{(p)}(r, r'; s). \quad (26)$$

Equation (25) is, in fact, the Green's equation for a 3D isotropic harmonic oscillator constrained to a centrifugal repulsion and with the shifted energy eigenvalue $\tilde{E}$.

Taking into account Eq. (22), we obtain:

$$\tilde{G}_J(r, r'; \tilde{E}) = (-i\hbar) \int_0^\infty e^{-s\beta} g_J^{(p)}(r, r'; \beta) d\beta. \quad (27)$$

By following Ref. 8, we can write the solution of Eq. (25) as Schwinger's integral representation [9]:

$$\begin{aligned} \tilde{G}_J(r, r'; \tilde{E}) &= \frac{m\omega}{2\hbar} \sqrt{rr'} \int_0^\infty dt \exp\left(\frac{i}{\hbar} \tilde{E}t\right) \frac{\sqrt{z}}{1-z} I_{\alpha_J} \left(\frac{m\omega}{\hbar} rr' \frac{\sqrt{z}}{1-z} \right) \\ &\times \exp\left[-\frac{m\omega}{4\hbar} (r^2 + r'^2) \frac{1+z}{1-z} \right], \end{aligned} \quad (28)$$

where we have used the notations:

$$z = \exp(-i\omega t), \quad (29)$$

$$\alpha_J = \sqrt{\frac{1}{4} + \left(\frac{m\omega}{2\hbar} r_J^2\right)^2} = \sqrt{\left(J + \frac{1}{2}\right)^2 + \left(\frac{m\omega}{2\hbar} r_0^2\right)^2} \quad (30)$$

and $I_{\alpha_J}(\dots)$ are the modified Bessel functions.

With the following new notations:

$$x = \frac{m\omega}{2\hbar} r^2, \quad y = \frac{m\omega}{2\hbar} r'^2, \quad (31)$$

Eq. (28) becomes:

$$\begin{aligned} \tilde{G}_J(r, r'; \tilde{E}) &= \frac{m\omega}{2\hbar} \sqrt{rr'} \int_0^\infty dt \exp\left(\frac{i}{\hbar} \tilde{E}t\right) \\ &\times z^{(\alpha_J+1)/2} \left[\frac{z^{-\alpha_J/2}}{1-z} I_{\alpha_J} \left(\frac{2\sqrt{xyz}}{1-z} \right) \exp\left(-\frac{x+y}{2} \frac{1+z}{1-z}\right) \right]. \end{aligned} \quad (32)$$

In this appearance, the quantity in the square brackets can be transformed using the Hille-Hardy relation [10]:

$$\sum_{v=0}^{\infty} \frac{v! L_v^\alpha(x) L_v^\alpha(y)}{\Gamma(\alpha+v+1)} z^v = \frac{(xyz)^{-\alpha/2}}{1-z} \exp\left(-z \frac{x+y}{1-z}\right) I_\alpha\left(2 \frac{\sqrt{xyz}}{1-z}\right), \quad (33)$$

where $L_v^\alpha(\dots)$ are Laguerre's polynomials. We obtain:

$$\begin{aligned} \tilde{G}_J(r, r'; \tilde{E}) &= \frac{m\omega}{2\hbar} \sqrt{rr'} \exp\left(-\frac{x+y}{2}\right) (xy)^{\alpha_J/2} \\ &\times \sum_{v=0}^{\infty} \frac{v!}{\Gamma(\alpha_J+v+1)} L_v^{\alpha_J}(x) L_v^{\alpha_J}(y) \int_0^\infty dt \exp\left(-i \left[\omega \left(\frac{\alpha_J+1}{2} + v \right) - \frac{\tilde{E}}{\hbar} \right] t\right). \end{aligned} \quad (34)$$

Integration over the variable t leads to the expression

$$\begin{aligned} \tilde{G}_J(r, r'; \tilde{E}) &= (-i\hbar) \frac{m\omega}{2\hbar} \sqrt{rr'} (xy)^{\alpha_J/2} \exp\left(-\frac{x+y}{2}\right) \\ &\times \sum_{v=0}^{\infty} \frac{v! L_v^{\alpha_J}(x) L_v^{\alpha_J}(y)}{\Gamma(\alpha_J+v+1)} \frac{1}{\left[\frac{1}{2}(\alpha_J+1) + v\right] \hbar\omega - \tilde{E}}. \end{aligned} \quad (35)$$

We use this expression of the PHO Green's function for obtaining the corresponding radial density matrix in coordinate representation (10) and, finally, the global density matrix (9).

By using Eq. (22), the inverse Laplace transform of the radial Green's function $G_J^{(p)}(r, r'; s)$ can be obtained by means of the residuum theorem:

$$g_J^{(p)}(r, r'; \beta) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} G^{(p)}(r, r'; s) e^{s\beta} ds = \sum_{n=1}^N \text{Res}_n \left[G^{(p)}(r, r'; s) e^{s\beta} \right]. \quad (36)$$

So, we obtain, according to Eqs. (24) and (26):

$$g_J^{(p)}(r, r'; \beta) = \frac{m\omega}{2\hbar} \sqrt{rr'} (xy)^{\alpha_J/2} \exp\left(-\frac{x+y}{2}\right) \times \sum_{v=0}^{\infty} \frac{v! L_v^{\alpha_J}(x) L_v^{\alpha_J}(y)}{\Gamma(\alpha_J + v + 1)} \sum_{n=1}^N \text{Res}_n \left[\frac{e^{s\beta}}{\left[\frac{1}{2}(\alpha_J + 1) + v\right] \hbar\omega + s - \frac{1}{4}m\omega^2 r_J^2} \right]. \quad (37)$$

The function into the square brackets has a single simple pole with respect to the variable $s = -\epsilon_{vJ}$:

$$s = -\left[\left(\frac{1}{2}(\alpha_J + 1) + v\right) \hbar\omega - \frac{1}{4}m\omega^2 r_J^2\right] = -\left(E_{vJ}^{(p)} - E_{0J}^{(p)}\right), \quad (38)$$

which, on one hand, leads to the correct energy eigenvalues for PHO [1]:

$$E_{vJ}^{(p)} = \hbar\omega \left(v + \frac{1}{2}\right) + \frac{1}{2}\hbar\omega\alpha_J - \frac{1}{4}m\omega^2 r_0^2 \quad (39)$$

and, on the other hand, Eq. (37) becomes:

$$g_J^{(p)}(r, r'; \beta) = \frac{m\omega}{2\hbar} \sqrt{rr'} \exp\left[\beta \left(\frac{m\omega^2}{4} r_J^2 - \frac{\alpha_J + 1}{2} \hbar\omega\right)\right] \times (xy)^{\alpha_J/2} \exp\left(-\frac{x+y}{2}\right) \sum_{v=0}^{\infty} \frac{v! L_v^{\alpha_J}(x) L_v^{\alpha_J}(y)}{\Gamma(\alpha_J + v + 1)} (e^{\beta\hbar\omega})^v. \quad (40)$$

When we are again using the Hille-Hardy relation (33) and Eq. (31), we finally obtain:

$$g_J^{(p)}(r, r'; \beta) = \exp\left(\beta \frac{m\omega^2}{4} r_J^2\right) \frac{1}{\sinh\left(\frac{1}{2}\beta\hbar\omega\right)} \frac{m\omega}{2\hbar} \sqrt{rr'} \times \exp\left[-\frac{m\omega}{4\hbar} (r^2 + r'^2) \coth\left(\frac{1}{2}\beta\hbar\omega\right)\right] I_{\alpha_J} \left(\frac{m\omega/(2\hbar) rr'}{\sinh\left(\frac{1}{2}\beta\hbar\omega\right)}\right). \quad (41)$$

According to Eq. (20), the radial density matrix $\rho_J^{(p)}(r, r'; \beta)$ is

$$\rho_J^{(p)}(r, r'; \beta) = \exp\left(\beta \frac{m\omega^2}{4} r_0^2\right) \frac{1}{\sinh\left(\frac{1}{2}\beta\hbar\omega\right)} \frac{m\omega/(2\hbar)}{\sqrt{rr'}} \times \exp\left[-\frac{m\omega}{4\hbar} (r^2 + r'^2) \coth\left(\frac{1}{2}\beta\hbar\omega\right)\right] I_{\alpha_J} \left(\frac{m\omega/(2\hbar) rr'}{\sinh\left(\frac{1}{2}\beta\hbar\omega\right)}\right). \quad (42)$$

This expression is the same as the previous obtained results in Ref. 11, where the starting point was Eq. (10).

By using an original method, involving the properties of Legendre polynomials and Bessel functions, in Ref. 3 we have restricted the expression (9) for the global density matrix and we have obtained the following result:

$$\rho^{(p)}(\vec{r}, \vec{r}'; \beta) = \rho^{(0)}(\vec{r}, \vec{r}'; \beta) \sqrt{\frac{(1 - 2\lambda \cos \gamma + \lambda^2) \sinh(\frac{1}{2}\beta\hbar\omega)}{\frac{m\omega}{4\hbar} rr' \sin^2 \gamma}} \times \sum_{j=0}^{\infty} \frac{\lambda^j}{\Gamma(\alpha_j + \frac{1}{2})} \left(\frac{m\omega}{4\hbar} \frac{rr' \sin^2 \gamma}{\sinh(\frac{1}{2}\beta\hbar\omega)} \right)^{\alpha_j}. \quad (43)$$

Here we have evinced the global density matrix of the isotropic 3D harmonic oscillator of the same mass m and the frequency $\omega_0 = \omega/2$:

$$\rho^{(0)}(\vec{r}, \vec{r}'; \beta) = \left(\frac{m\omega_0}{2\pi\hbar} \right)^{3/2} \frac{1}{[\sinh(\beta\hbar\omega_0)]^{3/2}} \times \exp \left(-\frac{m\omega_0}{2\hbar} \left[(r^2 + r'^2) \coth(\beta\hbar\omega_0) - \frac{2 \cos \gamma}{\sinh(\beta\hbar\omega_0)} rr' \right] \right). \quad (44)$$

The dimensionless parameter $|\lambda| < 1$ characterizes the degree of anharmonicity and the index (0) refers to the corresponding quantities of the harmonic oscillator.

3 Conclusions

In the present paper we have obtained the Green's function for the pseudoharmonical oscillator potential (PHO), which is used for expressing the corresponding density matrix in the coordinate (position) representation.

The used method is a hybrid one, based on the Laplace transformation and the "traditional" Green's function techniques. By transforming the initial PHO Hamiltonian, we get to a Green's equation, which has the same form as that for the Morse oscillator, from Ref. 8. So, it was possible to use the solution obtained in Ref. 8, as Schwinger's integral representation, for our problem, i.e. for the PHO Green's function.

The final expression for the density matrix (43) corresponds to our expression in Refs. 3 and 11, but it's obtained in another way. Even if this result is not new, the method for obtaining the density matrix via the corresponding Green's function can be, also, applied to a class of exactly solvable potentials. The advantage of the presented method consists in its simplicity in comparison with other methods (e.g. the Feynman's path integrals method [6] or the shape invariance method [12]).

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