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ALGEBRAIC TREATMENT OF THE MORSE POTENTIAL

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The Green's function for the Morse potential is calculated in the so(2,1) algebraic approach, using the Baker-Campbell-Hausdorff formulas.

Ever since the first notable success of the algebraic method in the calculation of wave functions and of hydrogen atom transition amplitudes [1], renewed interest for the algebraic approach has been emerging. Hence a certain number of potentials have been studied in the algebraic approach [2,3] and their Green's functions have been calculated. This algebraic method consists mainly in the transformation of the Schrödinger equation via a change of variables, in order to introduce generators satisfying a Lie algebra. When the evolution operator is expressed in terms of these generators in the configuration space, it is calculable for a certain class of potentials. In this paper, this algebraic approach is used to study the Morse potential defined as :

$$V(x) = A\,e^{-2ax} - B\,e^{-ax}, \tag{1}$$

where A, B and a are positive constants.

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This Morse potential has been very useful in molecular and nuclear physics. In a generalized separable and nonlocal form, it has once been used as a model for Nucleon-Nucleon [4] and P ion-Nucleon [5] interactions. The path integral solution to the problem can be found in the literature [6,7]. Two solutions used to be agreed on via the introduction of an auxiliary time-variable. A disagreement about expressions of the Green's function related to this potential and requiring a mathematical clarification [8] can nevertheless be noticed. This problem has been solved very recently [9].

The energy spectrum, propagator and Green's function have also been obtained in the phase-space approach of Weyl-Wigner-Moyal [10] . In the algebraic so (2,1) approach, the Green's function can be obtained in a direct and nice manner. Indeed, let G(x,x';E) be the Green's function which is solution of the differential equation :

$$(H-E)G(x,x';E) = -\hbar i\delta(x-x'), \qquad (2)$$

where $H(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$, is the hamiltonian of the particle and E its energy.

The transformation $\xi = \exp\left(-\frac{ax}{2}\right)$, then gives

$$\left(\widetilde{H}-\widetilde{E}\right)\widetilde{G}\left(\xi,\xi';\widetilde{E}\right) = -\hbar i\delta\left(\xi-\xi'\right), \qquad (3)$$

where

$$\widetilde{G}\left(\xi,\xi';\widetilde{E}\right) = \frac{2}{a}\left[\xi\xi'\right]^{1/2} G\left(x,x';E\right). \qquad (4)$$

The dynamics of the physical system is then governed by the new hamiltonian

$$\widetilde{H}(\xi,) = -\frac{\hbar^2}{2M}\left(\frac{d^2}{d\xi^2} - \frac{\mu(\mu-1)}{\xi^2}\right) + \frac{1}{2}M\widetilde{\omega}^2\xi^2, \qquad (5)$$

where $M = \frac{4m}{a^2}$, $\tilde{\omega}^2 = \frac{2A}{M}$, $\mu = \frac{1}{2} + \left(-\frac{2ME}{\hbar^2}\right)^{1/2}$, (6)

and $B = \tilde{E}$ is the pseudo-energy.

Expression (5) is the hamiltonian of a harmonic oscillator with a constant frequency, constrained to a centrifugal repulsion.

Besides, it is well known that the radial Coulombian system can be shown equivalent to the radial oscillator [9], with the help of a simple $r = \xi^2$ transformation. Consequently the Morse potential and the radial Coulombian system are equivalent and accept the same group dynamics.

It is easy to see that one can introduce the three following generators

$$T_1(\xi) = -\frac{\hbar^2}{2M}\left[\frac{\partial^2}{\partial\xi^2} - \frac{\mu(\mu-1)}{\xi^2}\right], \quad T_2(\xi) = -\frac{i}{2}\left(\xi\frac{\partial}{\partial\xi} + \frac{1}{2}\right), T_3(\xi) = \frac{M}{4\hbar^2}\xi^2, \tag{7}$$

satisfying the Lie algebra :

$$[T_1,T_2] = -iT_1, [T_2,T_3] = -iT_3, \text{ and } [T_1,T_3] = -iT_2 \tag{8}$$

The operator $\tilde{H}(\xi)$ can readily be expressed in terms of these generators :

$$\tilde{H}(\xi) = T_1(\xi) + 2\tilde{\omega}^2\hbar^2 T_3(\xi). \tag{9}$$

Being a linear combination of the generators T_i, $\tilde{H}(\xi)$ shows, as expected, a dynamical symmetry so (2,1) [11]. Expressed in Schwinger's integral representation [12] the solution of the differential equation (3), can be written as follows

$$G(\xi,\xi';\tilde{E}) = \int_0^\infty ds \exp\left[-\frac{i}{\hbar}\left(\tilde{H} - \tilde{E} - io\right)s\right]\delta(\xi-\xi') =$$

$$= \int_0^\infty ds \exp\left[\frac{i}{\hbar}\tilde{E}s\right]\exp\left\{\frac{-is}{\hbar}\left[T_1(\xi) + 2\hbar^2\tilde{\omega}^2 T_3(\xi)\right]\right\}\delta(\xi-\xi'). \tag{10}$$

The derivation of the Green's function in the algebraic approach, has been replaced by the calculation of the Kernel

$$P(\xi,\xi';s)=\exp\left\{\frac{-is}{\hbar}\left[T_1(\xi)+2\hbar^2\tilde{\omega}^2T_3(\xi)\right]\right\}\delta(\xi-\xi'). \qquad (11)$$

We can achieve this calculation thanks to the following two Baker-Campbell-Hausdorff (BCH) formulas :

$$\exp\left\{\frac{-is}{\hbar}\left[T_1+2\hbar^2\tilde{\omega}^2T_3\right]\right\}=\exp(-iaT_3)\exp(-ibT_2)\exp(-icT_1) , \qquad (12)$$

where

$$a=2\hbar\tilde{\omega}\tan(\tilde{\omega}s) , \qquad (13a)$$

$$b=2\mathrm{Ln}\left(\cos(\tilde{\omega}s)\right) , \qquad (13b)$$

$$c=\frac{1}{\hbar\tilde{\omega}}\tan(\tilde{\omega}s) , \qquad (13c)$$

and

$$\exp(-i\alpha T_3)\exp(-i\beta T_2)\exp(-i\gamma T_1)=\exp(-icT_1)\exp(\lambda T_3) , \qquad (14)$$

with

$$\alpha=\frac{i\lambda}{1-\frac{i\lambda c}{2}} \quad , \quad \beta=2\mathrm{Ln}\left(1-\frac{i\lambda c}{2}\right) \quad , \quad \gamma=\frac{c}{1-\frac{i\lambda c}{2}} \qquad (15)$$

Both formulas can be easily checked within the frame of another realization of the algebra, which may well be chosen as finite, for instance expressing T_i generators versus the Pauli matrices σ_i :

$$T_1=\frac{\sigma_1-i\sigma_2}{2\sqrt{2}} \quad , \quad T_2=-\frac{i\sigma_3}{2} \quad , \quad T_3=\frac{\sigma_1+i\sigma_2}{2\sqrt{2}} . \qquad (16)$$

In order to calculate (11), we set

$$\delta(\xi-\xi')=\frac{M}{2\hbar^2}\frac{\xi^{\mu}\xi'^{1-\mu}}{2i\pi}\int_{-i\infty+\delta}^{+i\infty+\delta}d\lambda\,\exp\left\{\frac{M\lambda}{4\hbar^2}\left(\xi^2-\xi'^2\right)\right\} , \quad \delta<0. \qquad (17)$$

By using (12, 14, 17), the kernel (11) now reads

$$P(\xi,\xi';s) = \frac{M}{2\hbar^2}\xi'^{1-\mu}\exp(-iaT_3)\exp(-ibT_2)\frac{1}{2i\pi}\int_{-i\infty+\delta}^{+i\infty+\delta} d\lambda\,\exp\left(-\frac{M}{4\hbar^2}\xi'^2\lambda\right)\exp(-icT_1)\exp\left(\frac{M}{4\hbar^2}\xi^2\lambda\right)\xi^{\mu} =$$

$$= \frac{M}{2\hbar^2}\xi'^{1-\mu}\exp(-iaT_3)\exp(-ibT_2)\frac{1}{2i\pi}\int_{-i\infty+\delta}^{+i\infty+\delta} d\lambda\,\exp\left(-\frac{M}{4\hbar^2}\xi'^2\lambda\right)\exp(-icT_1)\exp(\lambda T_3)\,\xi^{\mu} = \qquad (18a)$$

$$= \frac{M}{2\hbar^2}\xi'^{1-\mu}\exp(-iaT_3)\exp(-ibT_2)\frac{1}{2i\pi}\int_{-i\infty+\delta}^{+i\infty+\delta} d\lambda\,\exp\left(\frac{-M}{4\hbar^2}\xi'^2\lambda\right)\exp(-i\alpha T_3)\exp(-i\beta T_2)\exp(-i\gamma T_1)\,\xi^{\mu} = \qquad (18b)$$

$$= \frac{M}{2\hbar^2}\xi'^{1-\mu}\exp(-iaT_3)\exp(-ibT_2)\xi^{\mu}\frac{1}{2i\pi}\int_{-i\infty+\delta}^{+i\infty+\delta} d\lambda\,\frac{\exp\left\{\frac{M}{2\hbar^2}\left(\frac{-\lambda\xi'^2}{2}+\frac{\lambda\xi^2}{2-i\lambda c}\right)\right\}}{\left(1-\frac{i\lambda c}{2}\right)^{\mu+1/2}} = \qquad (18c)$$

$$= \frac{-iM}{\hbar^2 c}\exp(-iaT_3)\exp(-ibT_2)\left[(\xi'\xi)^{1/2}\, I_{\mu-1/2}\left(\frac{M\xi'\xi}{i\hbar^2 c}\right)\exp\left\{\frac{iM}{2\hbar^2 c}\left(\xi^2+\xi'^2\right)\right\}\right] = \qquad (18d)$$

$$= \frac{-iM}{\hbar^2 c}\exp\left(-\frac{iaM}{4\hbar^2}\xi^2\right)\exp\left(-\frac{b}{2}\right)(\xi'\xi)^{1/2}\, I_{\mu-1/2}\left(\frac{M\xi'\xi}{i\hbar^2 c e^{b/2}}\right)\exp\left\{\frac{iM}{2\hbar^2 c}\left(e^{-b}\xi^2+\xi'^2\right)\right\} = \qquad (18e)$$

$$= \frac{-iM\tilde{\omega}}{\hbar\sin(\tilde{\omega}s)}(\xi'\xi)^{1/2}\, I_{\mu-1/2}\left(\frac{M\tilde{\omega}\xi'\xi}{i\hbar\sin(\tilde{\omega}s)}\right)\exp\left\{\frac{iM\tilde{\omega}}{2\hbar}\left(\xi^2+\xi'^2\right)\cot(\tilde{\omega}s)\right\}. \qquad (18f)$$

The choice of the form of the Dirac delta distribution is dictated by the desire to obtain the simple following result :

$$\exp(-i\gamma T_1)\xi^{\mu} = \left(1 - i\gamma T_1 + \frac{1}{2!}(-i\gamma T_1)^2 + \dots\right)\xi^{\mu} = \xi^{\mu}\ .$$

Moreover we have used the formula

$$\exp(-i\beta T_2)\,f(\xi) = \exp\left\{-\frac{\beta}{2}\left[\xi\frac{\partial}{\partial\xi}+\frac{1}{2}\right]\right\}f(\xi) = \exp\left(-\frac{\beta}{4}\right)\exp\left[-\frac{\beta}{2}\frac{\partial}{\partial \mathrm{Ln}\xi}\right]f(\xi) =$$

$$= \exp\left(-\frac{\beta}{4}\right)\exp\left[-\frac{\beta}{2}\frac{\partial}{\partial u}\right]f(e^u) =$$

$$= \exp\left(-\frac{\beta}{4}\right) f(e^{u-\beta/2}) = \exp\left(-\frac{\beta}{4}\right) f(e^{-\beta/2}\xi) , \qquad (19)$$

when going over from eq. (18b) to (18c) and (18d) to (18e).

We calculate the integral contained within the eq. (18c) thanks to the Residue Theorem, by decomposing the $\frac{\lambda}{2-i\lambda c}$ factor and by expanding in a series the term in ξ^2 from the exponential function.

We used the following definitions for the first and second kind Bessel functions $J_\mu(x)$ and $I_\mu(x)$ [13, 14],

$$J_\mu(x) = \left(\frac{x}{2}\right)^\mu \sum_{n=0}^{\infty} \frac{\left(-x^2/4\right)^n}{n!\,\Gamma(n+\mu+1)} = \exp\left(i\frac{\pi}{2}\mu\right) I_\mu(-ix) . \qquad (20)$$

By inserting (18f) into (10) and then into (4), and by setting $\nu = \mu - 1/2$, the Green's function is then given by

$$G(x,x';E) = \frac{-iM\tilde{\omega}a}{2\hbar}\int_0^\infty ds\, \exp\left[\frac{i}{\hbar}\tilde{E}s\right]\frac{1}{\sin(\tilde{\omega}s)} I_\nu\left(\frac{M\tilde{\omega}\xi\xi'}{i\hbar\sin(\tilde{\omega}s)}\right)\exp\left[\frac{iM\tilde{\omega}}{2\hbar}\left(\xi^2+\xi'^2\right)\cot(\tilde{\omega}s)\right]. \qquad (21)$$

By using Gradshteyn's formula [15], with $v > u$,

$$\int_0^\infty dq\, \frac{e^{-2\lambda q}}{\sinh(q)} I_\nu\left(\frac{(uv)^{1/2}}{\sinh(q)}\right)\exp\left[-\frac{1}{2}(u+v)\coth(q)\right] = \frac{\Gamma\left(\lambda+\frac{\nu}{2}+\frac{1}{2}\right)}{(uv))^{1/2}\Gamma(\nu+1)} M_{-\lambda,\frac{\nu}{2}}(u)\, W_{-\lambda,\frac{\nu}{2}}(v) , \qquad (22)$$

where $M_{-\lambda,\frac{\nu}{2}}(u)$ and $W_{-\lambda,\frac{\nu}{2}}(v)$ are the standard Whittaker functions, the Green's function becomes

$$G(x,x';E) = \frac{-a}{2i\tilde{\omega}}\,\frac{\Gamma\left(p+\frac{\nu}{2}+\frac{1}{2}\right)}{\Gamma(\nu+1)}\exp\left[\frac{1}{2}a(x+x')\right] M_{-p,\frac{\nu}{2}}\left(De^{-ax'}\right) W_{-p,\frac{\nu}{2}}\left(De^{-ax}\right), \qquad (23)$$

with $x > x'$ and $p = -\frac{\tilde{E}}{2\hbar\tilde{\omega}}$.

This result (21) agrees with the one given in ref. [6].

We succeeded in showing that the Green's function of the Morse potential can be calculated by the so(2,1) algebraic approach. Energies and wave functions may be inferred from the poles of this Green's function in the complex plane.

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