Turk J Phys
31 (2007) , 197 – 203.

Green Function of the Morse Potential Using Perturbation Series

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Received 31.05.2007

Abstract

We find the Green function of the Schrodinger equation for the Morse potential using perturbation series. By Fourier transformation on the end point of the perturbation series, and with some formulas for terms generating the perturbation series, we are able to derive the Green function of the problem.

Key Words: Morse potential, Green function, Propagator, Path integral, Perturbation series, Fourier transform.

1. Introduction

Most physical problems cannot be treated exactly. It then becomes then necessary to develop different methods of approximation allowing one to approach the exact result with an appropriate accuracy. The most important and popular approximation method for solving problems in quantum mechanics, is the perturbation theory in the Schroëdinger formalism. It provides us with an effective method to compute the approximate solutions of many problems which can not be solved exactly. As in standard quantum mechanics, the perturbation method can be developed in the path integral framework of quantum mechanics [1].

In the last few decades, perturbation expansion of the path integral has been used to give the exact Green's functions for delta-function potential problems [2–4], for non-relativistic Coulomb systems [5], for the relativistic problem by summing the delta-function perturbation series [6], and for the relativistic Coulomb problem [7]. In addition, the perturbative approach was successfully used for deriving the energy Green function for the inverse square potential [8], and recently for the step potential [9].

In this paper, we would like to add a further contribution to the perturbation method. This contribution, which has not been treated to our knowledge and in this context, concerns the energy Green function of a Morse system, for bound states (for which the energy is negative), via summing over the perturbation series. However, we must mention that the Green function of the Morse potential was calculated by different authors using the standard method in quantum mechanics [10], or a path integral framework [11–14].

2. Perturbation Series of the Morse Potential

Consider the classical Lagrangian with a unit mass ($m = 1$):

$$L(x, \dot{x}, t) = \frac{\dot{x}^2}{2} - V(x), \tag{1}$$

where

$$V(x) = V_0(\exp(-2x) - 2\exp(-x)),$$

and $V_0 > 0$ is the strength of the potential. The Feynman propagator is defined, taking $\hbar = 1$, by

$$K(x, T/x_0, 0) = \int\limits_{x(0)=x_0}^{x(T)=x} D[x(t)] \exp(i \int\limits_0^T L(x, \dot{x}, t)dt) \tag{2}$$

where $D[x(t)]$ is the formal measure on the path space. If we split the Lagrangian into the free part and the interaction part, we can show that the propagator takes the form

$$K(x, T/x_0, 0) = \sum_{n=0}^{\infty} (i)^n K_n(x, T/x_0, 0), \tag{3}$$

where

$$K_n(x, T/x_0, 0) = (-1)^n \int\limits_0^T dt_n \cdots \int\limits_0^{t_2} dt_1 \int\limits_{-\infty}^{+\infty} \cdots \int\limits_{-\infty}^{+\infty} \prod_{j=0}^{j=n} K_0(x_{j+1}, t_{j+1}/x_j, t_j) \prod_{j=1}^{j=n} V(x_j)dx_j \tag{4}$$

and $K_0(x_{j+1}, t_{j+1}/x_j, t_j)$ is the free particle propagator given by

$$K_0(x_{j+1}, t_{j+1}/x_j, t_j) = \left(\frac{1}{2i\pi(t_{j+1} - t_j)}\right)^{1/2} \exp(i(x_{j+1} - x_j)^2/2(t_{j+1} - t_j)). \tag{5}$$

Now we take the Fourier transform of $K_n(x, T/x_0, 0)$ on T as

$$G_n(x, x_0 : E) = G_n(x, x_0) = \int\limits_0^{\infty} K_n(x, T/x_0, 0) \exp(iET)dT, \tag{6}$$

which can be rewritten as

$$\begin{aligned} G_n(x, x_0) &= (-1)^n \int\limits_{-\infty}^{+\infty} \cdots \int\limits_{-\infty}^{+\infty} \prod_{j=0}^{j=n} G_0(x_{j+1}, x_j) \prod_{j=1}^{j=n} V(x_j)dx_j \\ &= (-1)^n \int\limits_{-\infty}^{+\infty} dx_n G_0(x, x_n)V(x_n) \prod_{j=0}^{j=n-1} G_0(x_{j+1}, x_j) \prod_{j=1}^{j=n-1} V(x_j)dx_j \\ &= -\int\limits_{-\infty}^{+\infty} dx_n G_0(x, x_n)V(x_n)G_{n-1}(x_n, x_0), \end{aligned} \tag{7}$$

where

$$\begin{aligned} G_0(x, x_n) &= \int\limits_0^{\infty} dT \cdot K_0(x, T : x_n, 0) \exp(iET) \\ &= \int\limits_0^{\infty} \sqrt{\frac{1}{2i\pi T}} dT \cdot \exp\left(iET + \frac{i}{2T}(x - x_n)^2\right), \end{aligned} \tag{8}$$

If we put $V(x)$ in the suitable form

$$V(x) = V_0(\exp(-2x) - 2\exp(-x)) = 4V_0 \sum_{s=1}^{s=2} (-1/2)^s \exp(-sx), \tag{9}$$

equation (7), using (8), becomes

$$G_n(x, x_0) = -4V_0 \sum_{s=1}^{s=2} (-1/2)^s \int_0^\infty \sqrt{\frac{1}{2i\pi T}} dT \cdot \exp(iET)$$

$$\int_{-\infty}^{\infty} dx_n \cdot \exp\left(-sx_n + \frac{i}{2T}(x - x_n)^2\right) G_{n-1}(x_n, x_0) = \tag{10}$$

$$-4V_0 \sum_{s=1}^{s=2} (-1/2)^s \exp(-sx) \int_0^\infty \sqrt{\frac{1}{2i\pi T}} dT \cdot \exp(iET)$$

$$\int_{-\infty}^{\infty} dx_n \cdot \exp\left(s(x - x_n) + \frac{i}{2T}(x - x_n)^2\right) G_{n-1}(x_n, x_0). \tag{11}$$

We now take the Fourier transform of $G_n(x, x_0)$ on the end point x:

$$\widetilde{G_n}(\omega, x_0) = \int_{-\infty}^{+\infty} dx \exp(i\omega x) G_n(x, x_0) =$$

$$-4V_0 \sum_{s=1}^{s=2} (-1/2)^s \int_0^\infty \sqrt{\frac{1}{2i\pi T}} dT \cdot \exp(iET) \int_{-\infty}^{+\infty} dx \exp((i\omega - s)x)$$

$$\int_{-\infty}^{\infty} dx_n \cdot \exp\left(s(x - x_n) + \frac{i}{2T}(x - x_n)^2\right) G_{n-1}(x_n, x_0). \tag{12}$$

We note here that the integrals over x and x_n have a convolution form whose calculation is easily performed:

$$\widetilde{G_n}(\omega, x_0) = -4V_0 \sum_{s=1}^{s=2} (-1/2)^s \int_0^\infty \sqrt{\frac{1}{2i\pi T}} dT \cdot \exp(iET)$$

$$\left[\int_{-\infty}^{+\infty} dx \exp(i\Omega x) \exp(sx + \frac{i}{2T} x^2)\right] \widetilde{G_{n-1}}(\Omega, x_0), \tag{13}$$

where $\Omega = \omega + is$. Knowing that the integral in the square brackets is equal to

$$\int_{-\infty}^{+\infty} dx \exp(i\omega x + \frac{i}{2T} x^2) = \sqrt{2i\pi T} \exp(-\frac{i\omega^2 T}{2}), \tag{14}$$

we find that

$$\widetilde{G_n}(\omega, x_0) = -4V_0 \sum_{s=1}^{s=2} (-1/2)^s \int_0^\infty dT \cdot \exp iT\left(E - \frac{\omega^2}{2}\right) \widetilde{G_{n-1}}(\Omega, x_0). \tag{15}$$

We are interested in the bound states for which E is negative ($E = -\varepsilon^2$); thus we now we perform the integral over T:

$$-2if_0(\omega) \equiv \int_0^\infty dT \cdot \exp iT\left(E - \frac{\omega^2}{2}\right) = \int_0^\infty dT \cdot \exp\left[-iT\left(\varepsilon^2 + \frac{\omega^2}{2}\right)\right] = \frac{-2i}{2\varepsilon^2 + \omega^2}. \tag{16}$$

After inserting the last formula in (15) we find, after summing over s in (15), a recurrence relation for $n \geq 1$:

$$\widetilde{G_n}(\omega, x_0) = -\, V_0 f_0(\omega)\left[\widetilde{G_{n-1}}(\omega + 2i, x_0) - 2\widetilde{G_{n-1}}(\omega + i, x_0)\right], \tag{17}$$

and for the lower order this last equation translates into

$$\widetilde{G_{n-1}}(\omega + i, x_0) = iV_0\left(\frac{2}{2\epsilon^2 + (\omega + i)^2}\right)\left[\widetilde{G_{n-2}}(\omega + 3i, x_0) - 2\widetilde{G_{n-2}}(\omega + 2i, x_0)\right] \tag{18}$$

and

$$\widetilde{G_{n-1}}(\omega + 2i, x_0) = iV_0\left(\frac{2}{2\epsilon^2 + (\omega + 2i)^2}\right)\left[\widetilde{G_{n-2}}(\omega + 4i, x_0) - 2\widetilde{G_{n-2}}(\omega + 3i, x_0)\right], \tag{19}$$

and so on. If we continue the recurrence to the lower orders, we find the expression of $\widetilde{G_0}(\omega + ni, x_0)$

$$\begin{aligned} \widetilde{G_0}(\omega + ni, x_0) &= \int_{-\infty}^{+\infty} dx \exp(i(\omega + ni)x) G_0(x, x_0) \\ &= -\left(\frac{2i}{2\varepsilon^2 + (\omega + ni)^2}\right) \exp(i\omega - n)x_0 \\ &= -2if_n(\omega) \exp(i\omega - n)x_0, \end{aligned} \tag{20}$$

where

$$f_n(\omega) = \frac{1}{2\varepsilon^2 + (\omega + ni)^2} \quad ; n = 1, 2 \ldots. \tag{21}$$

Then for $n = 1$ in (17), we find:

$$\widetilde{G_1}(\omega, x_0) = 2^2 V_0\ f_0(\omega) \exp(i\omega x_0)\left[f_2(\omega) \exp(-2x_0) - 2f_1(\omega) \exp(-x_0)\right]$$

and

$$\begin{aligned} \widetilde{G_2}(\omega, x_0) = {} & i2^3 V_0^2 f_0(\omega) \exp(i\omega x_0) \\ & [f_2(\omega) f_4(\omega) \exp(-4x_0) - 2f_2(\omega) f_3(\omega) \exp(-3x_0) \\ & -2f_1(\omega) f_3(\omega) \exp(-3x_0) + 4f_1(\omega) f_2(\omega) \exp(-2x_0)]\,; \end{aligned}$$

and in a similar way we obtain the other terms.

Hence, using the recurrence relation (17), we can show that each term $\widetilde{G_n}(\omega, x_0)$ is written as a sum of exponentials, $\exp(-kx_0)$, i.e.,

$$\widetilde{G_n}(\omega, x_0) = \sum_{k=n}^{k=2n} C_k(\omega) \exp(-kx_0), \tag{22}$$

since $\widetilde{G}(\omega, x_0)$ is of the form

$$\widetilde{G}(\omega, x_0) = \sum_{n=0}^{\infty} (i)^n \, \widetilde{G_n}(\omega, x_0).$$

We note [14] that the perturbation series of the propagator is not analytic but is uniformly absolutely convergent in the coupling constant for every compact set in the variables $x, t, x_0, t_0 = 0$. Then from (22), if we bring together all terms in power of $\exp(-x_0)$, we find

$$\widetilde{G}(\omega, x_0) = 2if_0(\omega) \exp(i\omega x_0) \left[\sum_{n=0}^{\infty} a_n(\omega) \exp(-nx_0) \right], \tag{23}$$

where the coefficients $a_n(\omega)$ satisfy a recurrence formula

$$a_n(\omega) = 2V_0 f_n(\omega) \left(2a_{n-1}(\omega) - a_{n-2}(\omega)\right), \tag{24}$$

or

$$\left(2\varepsilon^2 + \omega^2 - n^2 + 2ni\omega\right) a_n(\omega) = 2V_0(2a_{n-1}(\omega) - a_{n-2}(\omega)), \tag{25}$$

with $a_{-1} = 0$, $a_0 = -1$; $a_1(\omega) = -4V_0 f_1(\omega)$ etc. Noting the series in brackets in (23) by:

$$2if_0(\omega)F(X) = 2if_0(\omega) \sum_{n=0}^{\infty} a_n(\omega) X^n \equiv \widetilde{G}(\omega, x_0) \exp(-i\omega x_0), \tag{26}$$

we can check then that the series $F(X)$, the generating function of $a_n(\omega)$, satisfies the differential equation

$$X^2 F\text{"}(X) + X(1 - 2i\omega)F'(X) - \left(2\varepsilon^2 + \omega^2 - 4XV_0 + 2X^2 V_0\right) F(X) = 2\varepsilon^2 + \omega^2. \tag{27}$$

Then with (26) and (27), we find that $\widetilde{G}(\omega, X)$ must satisfy the differential equation

$$-\frac{1}{2}\frac{d}{dX}\left(X^2 \frac{d}{dX}\widetilde{G}(X)\right) + \left[V_0(X^2 - 2X) + \varepsilon^2\right] \widetilde{G}(X) = -iX^{-i\omega}. \tag{28}$$

We note that this equation is equivalent to those governing Green's function itself but written in a form where we have put $X = \exp(-x_0)$ and done the Fourier transform on the end point x, i.e.

$$\left[-\frac{1}{2}\frac{d^2}{dx_0^2} + V(x_0) + \varepsilon^2\right] G(x, x_0/E) = -i\delta(x_0 - x). \tag{29}$$

We will return to the homogeneous equation associate to (28), i.e.

$$-\frac{1}{2}\frac{d}{dX}\left(X^2 \frac{d}{dX}\widetilde{G}(X)\right) + \left[V_0(X^2 - 2X) + \varepsilon^2\right] \widetilde{G}(X) = 0, \tag{30}$$

which is an equation of the hypergeometric class with two linearly independent solutions

$$\breve{G}_1(X) = X^{-\frac{1}{2}} M_{\sqrt{2V_0}, \varepsilon\sqrt{2}} \left(2\sqrt{2V_0} X\right)$$

$$\breve{G}_2(X) = X^{-\frac{1}{2}} W_{\sqrt{2V_0},\varepsilon\sqrt{2}} \left(2\sqrt{2V_0}X\right),$$

where $M_{\alpha,\beta}$, $W_{\alpha,\beta}$ denote Whittaker's functions [15].

Here we can see clearly that the change of variable $X = \exp(-x)$ is the appropriate change of variable to transform equation (29) to a Hypergeometric class equation (i.e. relation (30)).

Then with the same trick as above ($X = \exp(-x)$), equation (30) is converted to the relation

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + V(x) + \varepsilon^2\right]\Psi = 0. \tag{31}$$

Then from the solutions of the equation (30) we can conclude that

$$G_1(x) = \exp(-\frac{x}{2}) M_{\sqrt{2V_0},\varepsilon\sqrt{2}} \left(2\sqrt{2V_0}\exp(-x)\right)$$

$$G_2(x) = \exp(-\frac{x}{2}) W_{\sqrt{2V_0},\varepsilon\sqrt{2}} \left(2\sqrt{2V_0}\exp(-x)\right)$$

are two linearly independent solutions of the equation (31) which satisfy the conditions:

$$\lim_{x\to+\infty} G_1(x) = 0 \quad ; \quad \lim_{x\to-\infty} G_2(x) = 0$$

Then according to some results in [16] we know that the Green function of the equation (31), which is our solution of the equation (29), i.e. our initial Green function, is given in the following form:

$$G(x,y) = \begin{cases} \frac{G_2(y)G_1(x)}{W} & si \;\; y < x \\ \frac{G_2(x)G_1(y)}{W} & si \;\; x < y \end{cases}$$

where for equation (31) W is the Wronskian of $G_1,\ G_2$.

With some properties of the Whittaker functions [17], we find that

$$W = \frac{2\sqrt{2V_0}\Gamma\left(1+2\sqrt{-2E}\right)}{\Gamma\left(\frac{1}{2}+\sqrt{-2E}+\sqrt{2V_0}\right)}.$$

Finally the Green function takes the form

$$\begin{aligned} G(x,y) \quad = \quad & \frac{\Gamma\left(\frac{1}{2}+\sqrt{-2E}+\sqrt{2V_0}\right)}{2\sqrt{2V_0}\Gamma\left(1+2\sqrt{-2E}\right)} \exp\frac{1}{2}(x+y) \,. \\ & \Big\{\Theta(x-y)\, W_{\sqrt{2V_0},\sqrt{-2E}}\left(2\sqrt{2V_0}\exp(-y)\right) M_{\sqrt{2V_0},\sqrt{-2E}}\left(2\sqrt{2V_0}\exp(-x)\right) + \\ & \Theta(y-x)\, W_{\sqrt{2V_0},\sqrt{-2E}}\left(2\sqrt{2V_0}\exp(-x)\right) M_{\sqrt{2V_0},\sqrt{-2E}}\left(2\sqrt{2V_0}\exp(-y)\right)\Big\} \end{aligned}$$

where Θ denotes Heaviside's unit step function. A result was found earlier by different methods [11–14].

3. Discussion

In this work, we have added a further application, contributing to the perturbation method. This contribution concerns for first time the calculation of the energy Green's function of the Morse system by the perturbation series. This approach and the used method will, without any doubt, serve to bring another contribution to the non explored problems and we hope to stimulate further examples of applications in important problems of physics.

Acknowledgement

The authors thank Professor W. Koepf (Kassel University, Germany) for fruitful discussions, and their colleagues T. Boudjedaa and M. Benbitour for helpful comments.

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