ON THE EVOLUTION OPERATOR KERNEL FOR THE COULOMB AND COULOMB–LIKE POTENTIALS

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Abstract

With a help of the Schwinger — DeWitt expansion analytical properties of the evolution operator kernel for the Schrödinger equation in time variable $t$ are studied for the Coulomb and Coulomb-like (which behaves themselves as $1/|\vec{q}|$ when $|\vec{q}| \to 0$) potentials. It turned out to be that the Schwinger — DeWitt expansion for them is divergent. So, the kernels for these potentials have additional (beyond $\delta$-like) singularity at $t = 0$. Hence, the initial condition is fulfilled only in asymptotic sense. It is established that the potentials considered do not belong to the class of potentials, which have at $t = 0$ exactly $\delta$-like singularity and for which the initial condition is fulfilled in rigorous sense (such as $V(q) = -\frac{\lambda(\lambda-1)}{2} \frac{1}{\cosh^2 q}$ for integer $\lambda$).
1 Introduction

This paper continues the series of works [1, 2, 3] devoted to study of dependence of the evolution operator kernel for the Schrödinger equation on time interval \( t \) (especially, in vicinity of origin). We use for the kernel the Schwinger — DeWitt expansion [4, 5, 6] which in one-dimensional case reads

\[
\langle q', t \mid q, 0 \rangle = \frac{1}{\sqrt{2\pi it}} \exp \left\{ i \frac{(q' - q)^2}{2t} \right\} F(t; q', q),
\]

where

\[
F(t; q', q) = \sum_{n=0}^{\infty} (it)^n a_n(q', q).
\]

It was obtained [2] the estimate for the coefficients \( a_n \) which shows that this expansion is usually divergent, if there is no any cancellations of different contributions. Such cancellations really take place for some potentials, as it is established in [3]. For example, for the potential

\[
V(q) = -\frac{\lambda(\lambda - 1)}{2} \frac{1}{\cosh^2 q},
\]

the series (2) converges when \( \lambda \) is integer. Thus, for the most of the potentials the expansion (2) is divergent, but there exist the class of potentials for which this expansion is convergent at some discrete values of the coupling constant \( g \).

Divergence of expansion (2) shows that the function \( F \), which is really

\[
F(t; q', q) = \frac{\langle q', t \mid q, 0 \rangle_V}{\langle q', t \mid q, 0 \rangle_{V=0}}
\]

(subscribe \( V \) means that the kernel is taken for the potential \( V \)), has essential singularity at the point \( t = 0 \). Hence, \( F \) has no any meaning at this point and \( F \) tends to 1 for \( t \to 0 \) only in asymptotic sense.

Singularity of \( \langle q', t \mid q, 0 \rangle_{V=0} \) at \( t = 0 \) is acceptable and necessary, because

\[
\langle q', t = 0 \mid q, 0 \rangle_{V=0} = \delta(q' - q)
\]

in correspondence with initial condition for the kernel. But if \( F \) has additional singularity (namely this singularity is under consideration here), then one cannot say that

\[
\langle q', t = 0 \mid q, 0 \rangle_V = \langle q', t = 0 \mid q, 0 \rangle_{V=0} = \delta(q' - q).
\]
One can say only that
\[ \langle q', t \to +0 \mid q, 0 \rangle_V \to \langle q', t = 0 \mid q, 0 \rangle_{V=0} = \delta(q' - q) \] (7)
when \( t \) is real positive. Relation (7) has asymptotic character. Using it one can determine unambiguously evolution of the system, but asymptotic initial condition leads to appearance of divergences in different expressions. If one works with the potentials, for which the Schwinger — DeWitt expansion converges, e.g., with (3), then problem of divergence does not arise at all. One may assume in this connection that such potentials have emphasized meaning in quantum theory. This is why it is interesting to probe convergence of the expansion (2) for different frequently used potentials.

In present paper the Coulomb and Coulomb-like (the potentials which behave themselves as 1/|\( \vec{q} \)| when |\( \vec{q} \)| → 0 and are regular in some vicinity of the point |\( \vec{q} \)| = 0) potentials are under consideration. In the case of spherically symmetric potentials the three-dimensional kernel can be reduced to infinite sequence of one-dimensional ones for the effective potentials. For these kernels the technique developed in [3] is used.

## 2 The Schwinger — DeWitt expansion for spherically symmetric potentials

Let us consider the Schrödinger equation for the evolution operator kernel in three-dimensional space
\[ i \frac{\partial}{\partial t} \langle \vec{q}', t \mid \vec{q}, 0 \rangle = -\frac{1}{2} \sum_{i=1}^{3} \frac{\partial^2}{\partial q_i'^2} \langle \vec{q}', t \mid \vec{q}, 0 \rangle + V(\vec{q}') \langle \vec{q}', t \mid \vec{q}, 0 \rangle \] (8)
with initial condition
\[ \langle \vec{q}', t = 0 \mid \vec{q}, 0 \rangle = \delta(\vec{q}' - \vec{q}). \] (9)

Here and everywhere dimensionless values are used. If the potential \( V(\vec{q}) \) depends on \( q = |\vec{q}| \) only then it is more convenient to transfer to radial equation by means of representation
\[ \langle \vec{q}', t \mid \vec{q}, 0 \rangle = \sum_{l=0}^{\infty} \frac{2l + 1}{4\pi q'q} P_l(\cos \gamma) \langle q', t \mid q, 0 \rangle_t, \] (10)
where $\gamma$ is the angle between the vectors $\vec{q}'$ and $\vec{q}$, $P_l$ are the Legendre polynomials, $\langle q', t \mid q, 0 \rangle_l$ is "one-dimensional kernel" depending on absolute values of the vectors $\vec{q}'$, $\vec{q}$ and on integer number $l$. The variables $q'$, $q$ vary at the positive half-line.

Substitution of (10) into (8) gives equation

$$
i \frac{\partial}{\partial t} \langle q', t \mid q, 0 \rangle_l = -\frac{1}{2} \frac{\partial^2}{\partial q'^2} \langle q', t \mid q, 0 \rangle_l + \left( \frac{l(l+1)}{2} \frac{1}{q^2} + V(q') \right) \langle q', t \mid q, 0 \rangle_l,$$

which coincides in form with the one-dimensional Schrödinger equation for effective potential

$$U_l(q) = \frac{l(l+1)}{2} \frac{1}{q^2} + V(q).$$

The initial condition, as it is clear from consideration of the problem for $V(q) \equiv 0$, is to be taken in the form

$$\langle q', t = 0 \mid q, 0 \rangle_l = \delta(q' - q) - (-1)^l \delta(q' + q),$$

which provides correct behaviour of the solution at $q = 0$.

According to general procedure [5, 6, 3] we represent

$$\langle q', t \mid q, 0 \rangle_l = \frac{1}{\sqrt{2\pi it}} \exp \left\{ i \frac{(q' - q)^2}{2t} \right\} F_l^{(-)}(t; q', q) -$$

$$\frac{(-1)^l}{\sqrt{2\pi it}} \exp \left\{ i \frac{(q' + q)^2}{2t} \right\} F_l^{(+)}(t; q', q).$$

The equations for the functions $F_l^{(\pm)}$ are

$$i \frac{\partial F_l^{(\pm)}}{\partial t} = -\frac{1}{2} \frac{\partial^2 F_l^{(\pm)}}{\partial q'^2} + \frac{q' \pm q}{it} \frac{\partial F_l^{(\pm)}}{\partial q'} + U_l(q) F_l^{(\pm)}.$$  

Initial conditions are

$$F_l^{(\pm)}(t = 0; q', q) = 1.$$  

Here $F_l^{(\pm)}$ are defined for $q'$, $q > 0$. However, one can consider the analytical continuation into domain $q < 0$. It is necessary for this to come out into the complex plain of the variable $q$, because continuation along the real axis cannot be done so as the potential $U_l(q)$ and, hence, the functions $F_l^{(\pm)}$
have singularity at $q = 0$. It is clear from (15), (16) that $F_l^{(+)}(t; q', q) = F_l^{(-)}(t; q', -q)$ ($q > 0$). So, instead of two functions $F_l^{(+)}$ and $F_l^{(-)}$ one may consider only one function $F_l = F_l^{(-)}$, which is defined for $q$ varying along the hole real line. Instead of two equations (15) it is enough to consider only one equation for the function $F_l$ taking at (15) the lower sign.

Let us look for $F_l$ in the form
\[ F_l(t; q', q) = \sum_{n=0}^{\infty} (it)^n a^l_n(q', q). \] (17)

For the coefficient functions following relations are obtained
\[ a^l_0(q', q) = 1, \] (18)
\[ n a^l_n + (q' - q) \frac{\partial a^l_n}{\partial q'} = \frac{1}{2} \frac{\partial^2 a^l_{n-1}}{\partial q'^2} - U_l(q') a^l_{n-1}. \] (19)

The solutions of these equations can be represented as \[ a^l_n(q', q) = \int_0^1 \eta^{n-1} d\eta \left( \frac{1}{2} \frac{\partial^2}{\partial q'^2} - U_l(\bar{q}) \right) a^l_{n-1}(\bar{q}, q) \bigg|_{\bar{q} = q + (q' - q) \eta}. \] (20)

Another representation for $a^l_n$ can be derived starting from the expansion for the potential
\[ U_l(q') = \sum_{k=0}^{\infty} (q' - q)^k \frac{U_l^{(k)}(q)}{k!}, \] (21)
where
\[ U_l^{(k)}(q) \equiv \frac{d^k U_l(q)}{dq^k}. \]

It is possible to write for such $q'$, $q$, for which equation (21) takes place,
\[ a^l_n(q', q) = \sum_{k=0}^{\infty} (q' - q)^k b^n_{nk}(q). \] (22)

Then $b^l_{00}(q) = 1$ and for $n > 0$ one has recurrent relations
\[ b^l_{nk} = \frac{1}{n + k} \left[ (k + 1)(k + 2) b^l_{n-1,k+2} - \sum_{m=0}^{k} \frac{U_l^{(m)}(q)}{m!} b^l_{n-1,k-m} \right]. \] (23)
Note, that because of singularity of $U_l(q)$ at $q = 0$ the expansion (21) is not valid for $q < 0$. So, equations (23) can be used directly for calculation of $b_{nk}^l(q)$ only in the domain $q > 0$. However, for all potentials considered at present paper the expansion (17) is divergent. To prove divergence it is enough to show that only for one of two functions $F_l^{(+)}$ or $F_l^{(-)}$ and for one number $l$ the series of type (17) diverges. Therefore we will consider only positive $q$.

The relations obtained will be used for analysis of convergence of the Schwinger — DeWitt expansion for the Coulomb and Coulomb-like potentials.

3 The Coulomb potential

Let us consider the Coulomb potential

$$V(q) = \frac{\alpha}{q}.$$  \hfill (24)

The effective potential is

$$U_l(q) = \frac{l(l+1)}{2} \frac{1}{q^2} + \frac{\alpha}{q}.$$  \hfill (25)

"One-dimensional kernel" $\langle \bar{q}', t | q, 0 \rangle_l$ is the coefficient at the expansion (14) for the initial three-dimensional kernel $\langle \bar{q}', t | \bar{q}, 0 \rangle_l$ in the Legendre polynomials $P_l$. Therefore, if the expansion (17) in powers of $t$ for $\langle \bar{q}', t | q, 0 \rangle_l$ is divergent at least for any one value of $l$, then the Schwinger — DeWitt expansion for $\langle \bar{q}', t | \bar{q}, 0 \rangle_l$ is divergent too. We take $l = 0$. Then $U_0(q) = V(q) = \alpha/q$.

With a help of representation (20) one can consequently calculate the coefficient functions $a_n^0$. For example,

$$a_1^0(q', q) = -\frac{\alpha}{q' - q} \log \frac{q'}{q},$$  \hfill (26)

$$a_2^0(q', q) = \frac{\alpha^2}{2} \left( \frac{1}{q' - q} \log \frac{q'}{q} \right)^2 + \frac{\alpha}{(q' - q)^3} \log \frac{q'}{q} - \frac{\alpha}{2} \left( \frac{1}{q' - q} \right)^2$$

$$\times \left( \frac{1}{q'} + \frac{1}{q} \right),$$  \hfill (27)

etc.
Nevertheless, to evaluate behaviour of \( a_n^0 \) for \( n \to \infty \) it is more convenient to use (22), (23). Calculate derivatives

\[
V^{(m)}(q) = \frac{(-1)^m \alpha m!}{q^{m+1}}.
\]  

(28)

By means of (23) we find

\[
b_{1k}^0 = \frac{(-1)^{k+1}}{k+1} \frac{\alpha}{q^{k+1}},
\]

(29)

\[
b_{2k}^0 = \frac{(-1)^{k+1}}{k+2} \left[ \frac{(k+1)(k+2)}{2(k+3)} \frac{\alpha}{q^{k+3}} - \sum_{m=0}^{k} \frac{1}{m+1} \frac{\alpha^2}{q^{k+2}} \right],
\]

(30)

\[
b_{3k}^0 = \frac{(-1)^{k+1}}{k+3} \left[ \frac{(k+1)(k+2)(k+3)(k+4)}{2^2(k+4)(k+5)} \frac{\alpha}{q^{k+5}} - \frac{1}{2} \left( \frac{(k+1)(k+2)}{k+4} \sum_{m=0}^{k} \frac{1}{m+1} + \sum_{m=0}^{k} \frac{m+1}{m+3} \right) \frac{\alpha^2}{q^{k+4}} + \sum_{m=0}^{k} \frac{1}{m+2} \sum_{m'=0}^{m} \frac{1}{m'+1} \frac{\alpha^2}{q^{k+3}} \right].
\]

(31)

It is easy to understand that the coefficients \( b_{nk}^0 \) in this case have the following structure

\[
b_{nk}^0(q) = \sum_{j=1}^{n} (-1)^{k+j} C_{nk}^j \frac{\alpha^j}{q^{k+2n-j}},
\]

(32)

and besides the numerical coefficients \( C_{nk}^j \) and all partial contributions into them are positive. It means that for every \( m \) all contributions into coefficients in front of \( 1/q^m \) has the same sign and nothing cancellations do occur. In this case, as it follows from the analysis of representation (20) [2], the coefficients \( b_{nk}^0 \) and \( a_n^0 \) will increase as \( n! \) at \( n \to \infty \).

One can convinced of this directly from relations (23). Put \( k = 0 \) and calculate \( C_{n0}^1 \). It is obviously, that

\[
C_{n0}^1 = \frac{(n-1)!}{2^{n-1}(2n-1)} \sim n!
\]

(33)
Because the value $-C_{n0}^1$ is the coefficient in front of independent structure 
$(it)^n \Delta q^0/q^{2n+1}$ at the expansion (17), then its factorial growth means that $|a_n| \sim n!$ for $n \to \infty$.

Thus we established divergence of the Schwinger — DeWitt expansion for the Coulomb potential. This means that the initial condition (9) (or (13)) for the kernel cannot be fulfilled because of essential singularity of the solution of the Schrödinger equation at the point $t = 0$. So, the evolution operator kernel for the Coulomb potential exists only in asymptotic sense.

4 Other potentials with Coulomb-like singularity $1/|\vec{q}|$

Consider spherically symmetric potential of the form

$$V(q) = \frac{\alpha}{q} + f(q),$$

(34)

where $f(q)$ is regular in some vicinity of zero function, which can be represented at this domain by the convergent series

$$f(q) = \sum_{k=0}^{\infty} f_k q^k.$$  

(35)

For example, the Yukawa potential

$$V(q) = \frac{\alpha}{q} e^{-\beta q}$$

(36)

belongs to this class.

Analogously to previous section, to analyse the Schwinger — DeWitt expansion for the kernel $\langle \vec{q}', t \mid \vec{q}, 0 \rangle$ for convergence we consider "one-dimensional kernel" $\langle q', t \mid q, 0 \rangle_l$ for $l = 0$. Then the effective potential is $U_0(q) = V(q)$. The derivatives of the potential read

$$U_0^{(m)}(q) = V^{(m)}(q) = \frac{(-1)^m \alpha m!}{q^{m+1}} + \sum_{l=m}^{\infty} \frac{l!}{(l-m)!} f_l q^{l-m}.$$  

(37)

One can consequently determine all $b_{nk}^0$ from relations (23). For instance,

$$b_{1k}^0 = \frac{(-1)^{k+1}}{k+1} \frac{\alpha}{q^{k+1}} - \frac{1}{k+1} \sum_{l=k}^{\infty} \frac{l!}{k!(l-k)!} f_l q^{l-k},$$  

(38)
Consider the coefficients at the expansion of the function $F_0(t; q', q)$ in front of the structure $(it)^n \Delta q^0/q^{2n+1}$. One can see from (23) that these coefficients are equal to $-C^1_{n0}$, where $C^1_{n0}$ is determined so as in the case of the Coulomb potential by the formula (33). The contributions arising from adding of $f(q)$ to the Coulomb potential at (34) change the coefficients in front of the structures $(it)^n \Delta q^0/q^m$ only with $m < 2n + 1$. This means that factorial growth of $C^1_{n0}$ cannot be cancelled by anything. Hence, the Schwinger — DeWitt expansion for the potentials of type (34), so as for the Coulomb potential, is divergent. The kernels for such potentials exist only in asymptotic sense too.

Result of our research is following: it is established that for the Coulomb and Coulomb-like potentials the Schwinger — DeWitt expansion for the evolution operator kernel is divergent. So, the kernels for these potentials have additional (beyond $\delta$-like) singularity at $t = 0$. Hence, the initial condition (1) may be fulfilled only in asymptotic sense. The potentials considered do not belong to the class of potentials such as (3), for which the Schwinger — DeWitt expansion is convergent.
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